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LOGINID:SSPTATDH1621

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS	4	JUN 26	NUTRACEUT and PHARMAML no longer updated
NEWS	5	JUN 29	IMSCOPROFILE now reloaded monthly
NEWS	6	JUN 29	EPFULL adds Simultaneous Left and Right Truncation (SLART) to AB, MCLM, and TI fields
NEWS	7	JUL 09	PATDPAFULL adds Simultaneous Left and Right Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS	8	JUL 14	USGENE enhances coverage of patent sequence location (PSL) data
NEWS	9	JUL 27	CA/CAPLUS enhanced with new citing references
NEWS	10	JUL 16	GBFULL adds patent backfile data to 1855
NEWS	11	JUL 21	USGENE adds bibliographic and sequence information
NEWS	12	JUL 28	EPFULL adds first-page images and applicant-cited references
NEWS	13	JUL 28	INPADOCDB and INPAFAMDB add Russian legal status data
NEWS	14	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	15	AUG 17	CAS REGISTRY, the Global Standard for Chemical Research, Approaches 50 Millionth Registration Milestone
NEWS	16	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	17	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	18	AUG 24	CA/CAPLUS enhanced with legal status information for U.S. patents
NEWS EXPRESS	MAY 26 09	CURRENT WINDOWS VERSION IS V8.4, AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.	
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		

Enter NEWS followed by the item number or name to see news on that specific topic.

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and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:00:42 ON 01 SEP 2009

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.22

0.22

FILE 'REGISTRY' ENTERED AT 10:01:06 ON 01 SEP 2009

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STRUCTURE FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8

DICTIONARY FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

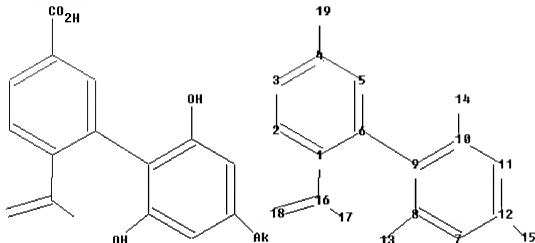
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\TDH PTA\Application Examination\Series 10\10 570737\STN\STN 10 570737
090109AA.str



```
chain nodes :
13 14 15 16 17 18 19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-16 4-19 6-9 8-13 10-14 12-15 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
8-13 10-14 12-15
exact bonds :
1-16 4-19 6-9 16-17 16-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

Match level :

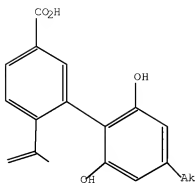
```
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS
```

L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> S L1
SAMPLE SEARCH INITIATED 10:01:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED      6 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   6 TO      266
PROJECTED ANSWERS:      0 TO      0
```

L2 0 SEA SSS SAM L1

```
=> S L1 SSS FUL
FULL SEARCH INITIATED 10:01:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      230 TO ITERATE
```

```
100.0% PROCESSED      230 ITERATIONS      1 ANSWERS
SEARCH TIME: 00.00.01
```

L3 1 SEA SSS FUL L1

```
=> S L1 SSS FULL
FULL SEARCH INITIATED 10:01:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      230 TO ITERATE
```

```
100.0% PROCESSED      230 ITERATIONS      1 ANSWERS
SEARCH TIME: 00.00.01
```

L4 1 SEA SSS FUL L1

```
=> D L4
```

```
L4  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2009 ACS on STN
RN  1027505-84-5  REGISTRY
ED  Entered STN:  12 Jun 2008
CN  INDEX NAME NOT YET ASSIGNED
MF  C25 H32 O4
SR  Other Sources
```

Database: ChemSpider (ChemZoo, Inc.)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> FILE CAPLUS
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
374.29	374.51

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:02:40 ON 01 SEP 2009
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FILE COVERS 1907 - 1 Sep 2009 VOL 151 ISS 10
FILE LAST UPDATED: 31 Aug 2009 (20090831/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> S L4
L5

0 L4

=> D HIS

(FILE 'HOME' ENTERED AT 10:00:42 ON 01 SEP 2009)

FILE 'REGISTRY' ENTERED AT 10:01:06 ON 01 SEP 2009

L1	STRUCTURE UPLOADED
L2	0 S L1
L3	1 S L1 SSS FUL
L4	1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:02:40 ON 01 SEP 2009

L5

0 S L4

=> S L3

L6 0 L3

=> FILE STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.50

376.01

FILE 'STNGUIDE' ENTERED AT 10:04:28 ON 01 SEP 2009

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_FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Aug 28, 2009 (20090828/UP).

=> FILE REGISTRY
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.42	376.43

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:08:07 ON 01 SEP 2009
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STRUCTURE FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8
DICTIONARY FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

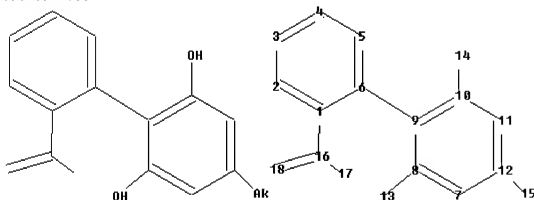
TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\TDH PTA\Application Examination\Series 10\10 570737\STN\STN 10 570737
090109AB.str



chain nodes :
13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-16 6-9 8-13 10-14 12-15 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
8-13 10-14 12-15
exact bonds :

1-16 6-9 16-17 16-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

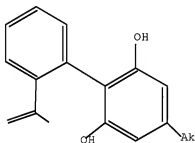
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L7 STRUCTURE UPLOADED

=> D

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L7 SSS SAM

SAMPLE SEARCH INITIATED 10:08:28 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5 TO 234

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> S L7 SSS FULL

FULL SEARCH INITIATED 10:08:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 89 TO ITERATE

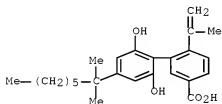
100.0% PROCESSED 89 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

L9 3 SEA SSS FUL L7

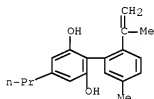
=> D L9 1-3

L9 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 1027505-84-5 REGISTRY
 ED Entered STN: 12 Jun 2008
 CN INDEX NAME NOT YET ASSIGNED
 MF C25 H32 O4
 SR Other Sources
 Database: ChemSpider (ChemZoo, Inc.)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 41408-26-8 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-propyl- (CA
 INDEX NAME)
 MF C19 H22 O2
 LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 39624-81-2 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA
 INDEX NAME)
 OTHER NAMES:
 CN Cannabinodiol
 MF C21 H26 O2
 LC STN Files: AGRICOLA, BEILSTEIN*, CA, CAPLUS, CASREACT, EMBASE,
 NAPRALERT, TOXCENTER

(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> FILE CAPLYS

'CAPLYS' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'REGISTRY'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

192.51

568.94

FILE 'CAPLUS' ENTERED AT 10:09:28 ON 01 SEP 2009

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FILE COVERS 1907 - 1 Sep 2009 VOL 151 ISS 10

FILE LAST UPDATED: 31 Aug 2009 (20090831/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/Caplus family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> S L9

L10 11 L9

=> D L10 1-11 IBIB ABS HITSTR

L10 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2009:91060 CAPLUS Full-text

DOCUMENT NUMBER: 151:97310

TITLE: PKS activities and biosynthesis of cannabinoids and flavonoids in Cannabis sativa L. plants

AUTHOR(S): Flores-Sanchez, Isvett Josefina; Verpoorte, Robert

CORPORATE SOURCE: Pharmacognosy Department/Metabolomics, Institute of Biology, Gorlaeus Laboratories, Leiden, 2300 RA, Neth.

SOURCE: Plant and Cell Physiology (2008), 49(12), 1767-1782
CODEN: PCPHA5; ISSN: 0032-0781

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

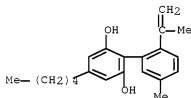
LANGUAGE: English

AB Polyketide synthase (PKS) enzymic activities were analyzed in crude protein exts. from cannabis plant tissues. Chalcone synthase (CHS, EC 2.3.1.74), stilbene synthase (STS, EC 2.3.1.95), phlorisovalerophenone synthase (VPS, EC 2.3.1.156), isobutyrophenone synthase (BUS) and olivetol synthase activities were detected during the development and growth of glandular trichomes on bracts. Cannabinoid biosynthesis and accumulation take place in these glandular trichomes. In the biosynthesis of the first precursor of cannabinoids, olivetolic acid, a PKS could be involved; however, no activity for an olivetolic acid-forming PKS was detected. Content analyses of cannabinoids and flavonoids, two secondary metabolites present in this plant, from plant tissues revealed differences in their distribution, suggesting a diverse regulatory control for these biosynthetic fluxes in the plant.

IT 39624-81-2, Cannabinodiol
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(polyketide synthase activities and biosynthesis of cannabinoids and flavonoids in Cannabis sativa plants)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2008:1383559 CAPLUS Full-text

DOCUMENT NUMBER: 149:555077

TITLE: Photocyclization of stilbenes and related molecules

AUTHOR(S): Mallory, Frank B.; Mallory, Clelia W.

CORPORATE SOURCE: Bryn Mawr Coll., Bryn Mawr, PA, USA

SOURCE: Organic Reactions (Hoboken, NJ, United States) (1984), 30, No pp. given
CODEN: ORHNBA
URL: <http://www3.interscience.wiley.com/cgi-bin/mrw/home/107610747/HOME>
John Wiley & Sons, Inc.

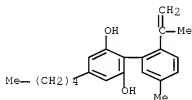
PUBLISHER: Journal; General Review; (online computer file)

DOCUMENT TYPE: English

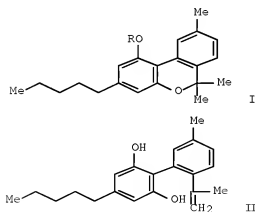
LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:555077

AB A review of the article Photocyclization of stilbenes and related mols.
 IT 39624-31-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Photocyclization of Stilbenes and Related Mols.)
 RN 39624-81-2 CAPLUS
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA
 INDEX NAME)

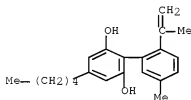


L10 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2008:532576 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 149:10131
 TITLE: A Cyclotrimerization Route to Cannabinoids
 AUTHOR(S): Teske, Jesse A.; Deiters, Alexander
 CORPORATE SOURCE: Department of Chemistry, North Carolina State
 University, Raleigh, NC, 27695-8204, USA
 SOURCE: Organic Letters (2008), 10(11), 2195-2198
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 149:10131
 GI



AB Three members of the cannabinoid class, cannabinol I (R = H), cannabinol Me ether I (R = Me), and cannabiodiol II, were synthesized using a microwave-mediated [2 + 2 + 2] cyclotrimerization reaction as the key step. This approach provides a high level of synthetic flexibility allowing for the facile synthesis of cannabinoid analogs.

IT 39624-81-2P, Cannabinodiol
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of cannabinoids via Rh-catalyzed microwave-mediated
 [2+2+2]-cyclootrimerization)
 RN 39624-81-2 CAPLUS
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA
 INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
 (2 CITINGS)
 REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN
 ACCESSION NUMBER: 2006:164717 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 144:226318
 TITLE: Methods for improving cognitive functioning
 INVENTOR(S): Coulston, Carissa Maree; Tennant, Christopher Charles;
 Perdices, Michael
 PATENT ASSIGNEE(S): Northern Sydney and Central Coast Area Health Service,
 Australia
 SOURCE: PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006017892	A1	20060223	WO 2005-AU1227	20050816
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: AU 2004-904641 A 20040816
 AB The present invention relates to methods for improving cognitive functioning
 in an individual suffering from a neuropsychiatric disorder associated with
 impaired cognitive functioning, the method comprising administering to the
 individual a therapeutically effective amount of cannabis, or at least one

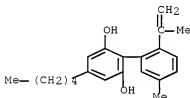
extract or constituent thereof, or administering to the individual a therapeutically effective amount of at least one agonist of a cannabinoid receptor. Frequent use of cannabis was shown to be a strong predictor of cognitive performance in schizophrenic subjects.

IT 39624-81-2, Cannabinodiol

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cannabis administration for improving cognitive functioning)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1986:83174 CAPLUS Full-text

DOCUMENT NUMBER: 104:83174

ORIGINAL REFERENCE NO.: 104:13093a,13096a

TITLE: Advanced high pressure liquid chromatography (HPLC) method for the analysis of cannabinoids in Cannabis sativa L

AUTHOR(S): Al-Hakawati, M. I.; Paris, M.

CORPORATE SOURCE: Lab. Pharmacogn., UER Sci. Pharm., Chatenay-Malabry, 92000, Fr.

SOURCE: Marihuana '84 [Eighty-Four], Proc. Oxford Symp. Cannabis (1985), Meeting Date 1984, 163-8. Editor(s): Harvey, D. J. IRL: Oxford, UK.
CODEN: 54PAAW

DOCUMENT TYPE: Conference

LANGUAGE: English

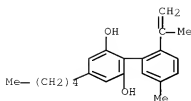
AB Major and minor cannabinoids in India hemp samples were identified and measured by chromatog. on a μ Bondapak C18 column with 0.02N H₂SO₄-1.6% THF in MeOH (21:97) at 1.8 mL/min, with eluate monitoring at 254 nm. This method separated 5 neutral and 3 acidic cannabinoids as well as 3 homologs with Pr side-chains. The method complimented TLC (silica gel, hexane-dioxane [8:2], Fast Blue Salt) and gas chromatog. (5% OV-1 on Chromapak, 200°, flame-ionization detection).

IT 39624-81-2

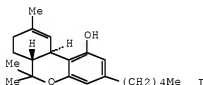
RL: BIOL (Biological study)
(detection and determination of, by gas chromatog. and HPLC and TLC)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)



L10 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1982:416578 CAPLUS Full-text
 DOCUMENT NUMBER: 97:16578
 ORIGINAL REFERENCE NO.: 97:2769a,2772a
 TITLE: Gas chromatographic and mass spectrometric studies on the metabolism and pharmacokinetics of Δ^1 -tetrahydrocannabinol in the rabbit
 AUTHOR(S): Harvey, D. J.; Leuschner, J. T. A.; Paton, W. D. M.
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK
 SOURCE: Journal of Chromatography (1982), 239, 243-50
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

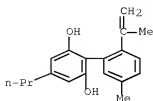


AB The in vivo hepatic metab. of Δ^1 -THC (I) [1972-08-3] was studied in the New Zealand white rabbit by a previously developed gas chromatog.-mass spectrometry (GC-MS) method. Sixteen metabolites were identified and shown to be present in different relative amts. compared with the hepatic metabolites of Δ^1 -THC produced by other species. The metabolic profile was also different from that reported from rabbit urine particularly with regard to the lower relative concns. of acidic metabolites in the liver. The pharmacokinetics of Δ^1 -THC was studied in the rabbit using the recently developed GC-MS method based on metastable ion monitoring. This revealed a terminal plasma Δ^1 -THC half life ranging from 34.16 to 59.30 h (mean 46.75 h) after a single dose and a THC fat/plasma ratio of 104-103:1.

IT 41408-26-8
 RL: ANT (Analyte); ANST (Analytical study)
 (determination of, by gas liquid chromatog.)

RN 41408-26-8 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-propyl- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L10 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1978:49835 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 88:49835
ORIGINAL REFERENCE NO.: 88:7861a,7864a
TITLE: Mass spectrometry of cannabinoids
AUTHOR(S): Vree, T. B.
CORPORATE SOURCE: Dep. Clin. Pharm., Radboudhosp., Nijmegen, Neth.
SOURCE: Journal of Pharmaceutical Sciences (1977), 66(10),
1444-50
CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The mechanism of fragmentation of cannabinoids to fragments m/e 314, 299, 271, 258, 246, 243, and 231 is given. Cannabidiol, cannabinodiol, cannabinol, Δ6- and Δ1-tetrahydrocannabinol, cannabichromene, cannabicyclol, derivs. with CSH11, Pr, and Me side chains, their Me ethers, and cis-trans and ortho-para isomers were analyzed by gas-liquid chromatog. (GLC)-mass spectrometry using different energies for fragmentation during GLC elution. Loss of Me, ring closure, and rotation, McLafferty rearrangement, retro Diels-Alder, internal protonation, isomerization and internal bond formation, and one-step fragmentation to m/e 231 are observed

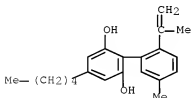
IT 39624-81-2

RL: PRP (Properties)

(mass spectrum of, mechanism of fragmentation of)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)

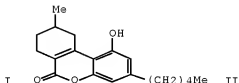
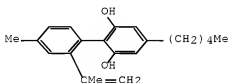


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

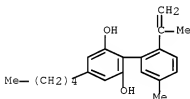
L10 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:502442 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 87:102442

ORIGINAL REFERENCE NO.: 87:16275a,16278a
 TITLE: Cannabinodiol: conclusive identification and synthesis of a new cannabinoid from Cannabis sativa
 Lousberg, Robert J. J. C.; Bercht, C. A. Ludwig; Van Ooyen, Ronald; Spronck, Hubertus J. W.
 AUTHOR(S):
 CORPORATE SOURCE: Org. Chem. Lab., Univ. Utrecht, Utrecht, Neth.
 SOURCE: Phytochemistry (Elsevier) (1977), 16(5), 595-7
 CODEN: PYTCAS; ISSN: 0031-9422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Cannabinodiol (I) was isolated from C. sativa and its structure detd. by
 synthesis from II and acid-catalyzed conversion into cannabinol.
 IT 39624-81-2P
 RL: PREP (Preparation)
 (from Cannabis sativa)
 RN 39624-81-2 CAPLUS
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA
 INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
 (2 CITINGS)

L10 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2009 ACS ON STN
 ACCESSION NUMBER: 1976:17576 CAPLUS Full-text
 DOCUMENT NUMBER: 84:17576
 ORIGINAL REFERENCE NO.: 84:2922h,2923a
 TITLE: Photochemical transformations of cannabinol
 AUTHOR(S): Bowd, Alexander; Swann, Donald A.; Turnbull, James H.
 CORPORATE SOURCE: Chem. Branch, R. Mil. Coll. Sci., Swindon, UK
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1975), (19), 797-8
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.

AB Irradn. of cannabinal (I) in EtOH gave the ring cleaved product II, which on further irradiation, underwent cyclodehydration to give the substituted phenanthrene III.

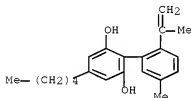
IT 39624-81-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and photochem. cyclodehydration of)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L10 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:119810 CAPLUS Full-text

DOCUMENT NUMBER: 78:119810

ORIGINAL REFERENCE NO.: 78:19221a,19224a

TITLE: Gas chromatography of cannabis constituents and their synthetic derivatives

AUTHOR(S): Vree, T. B.; Breimer, D. D.; Van Ginneken, C. A. M.; Van Rossum, J. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Nijmegen, Nijmegen, Neth.

SOURCE: Journal of Chromatography (1972), 74(2), 209-24

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

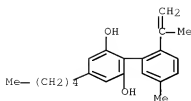
AB Based on the gas chromatog. and mass spectrometric anal. of 25 natural cannabinoids such as cannabidiol [13956-29-1], 1,6-tetrahydrocannabinol (I) [1972-08-3], and cannabinal [521-35-7], or 45 synthetic cannabinoid derivs. including resorcin-O,O-dimethyl [151-10-0] or orcinol [504-15-4], the retention times of groups of cannabinoids displayed a characteristic pattern. An increase in the side-chain of the aromatic ring, increased the retention time by a fixed amount, 42% per C atom. A shift in the position of the side chain of the aromatic ring from ortho to para increased the retention time by a factor of 1.3. The reduction of polarity by methylation and silylation decreased the retention time by a factor of 0.53. Side-chain branching increased the retention time 12%, and saturation of the double bond decreased the retention time by a factor of 0.80. The fictive retention of the cannabis constituents and synthetic derivs. were given.

IT 39624-81-2 41408-26-8

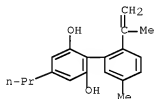
RL: ANT (Analyte); ANST (Analytical study) (detection of)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA INDEX NAME)



RN 41408-26-8 CAPLUS
 CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-propyl- (CA
 INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
 (1 CITINGS)

L10 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1973:119799 CAPLUS Full-text

DOCUMENT NUMBER: 78:119799

ORIGINAL REFERENCE NO.: 78:19217a,19220a

TITLE: Cannabinodiol, a new hashish constituent, identified
 by gas chromatography-mass spectrometry

AUTHOR(S): Van Ginneken, C. A. M.; Vree, T. B.; Breimer, D. D.;
 Thijssen, H. W. H.; Van Rossum, J. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Nijmegen, Nijmegen, Neth.

SOURCE: Proc. Int. Symp. Gas Chromatogr. Mass Spectrom. (1972)
 , 109-29. Editor(s): Frigerio, Alberto. Tamburini:
 Milan, Italy.

CODEN: 26IRAT

DOCUMENT TYPE: Conference

LANGUAGE: English

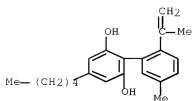
AB A new cannabinoid component in exts. of Nepalese hashish and Brazilian
 marihuana was discovered by comparing its properties in gas chromatog. and
 mass spectrometry with the properties of numerous cannabinol-like substances.
 A trivial name, cannabinodiol (I) [39624-81-2], was proposed for the newly
 discovered aromatic cannabidiol.

IT 39624-81-2

RL: BIOL (Biological study)
 (of hashish and marihuana)

RN 39624-81-2 CAPLUS

CN [1,1'-Biphenyl]-2,6-diol, 5'-methyl-2'-(1-methylethenyl)-4-pentyl- (CA
 INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

=> FILE STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	64.54	633.48
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-9.02	-9.02

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=> FILE STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.07	633.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.02

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=>

=> FILE REGISTRY
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
0.49	634.04

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
0.00	-9.02

CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8
DICTIONARY FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

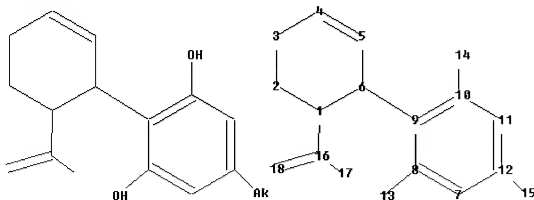
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

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Uploading C:\TDH PTA\Application Examination\Series 10\10 570737\STN\STN 10 570737
090109AC.str



chain nodes :
13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-16 6-9 8-13 10-14 12-15 16-17 16-18


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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-13 10-14 12-15
exact bonds :
1-16 6-9 16-17 16-18
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

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Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

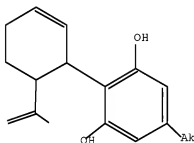
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L11 STRUCTURE UPLOADED

=> D

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L11 SSS SAMPLE

SAMPLE SEARCH INITIATED 10:18:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 229 TO ITERATE

100.0% PROCESSED 229 ITERATIONS

7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 3673 TO 5487

PROJECTED ANSWERS: 7 TO 298

L12 7 SEA SSS SAM L11

=> S L11 SSS FULL

FULL SEARCH INITIATED 10:18:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4548 TO ITERATE

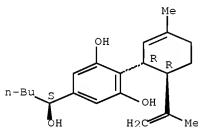
100.0% PROCESSED 4548 ITERATIONS

228 ANSWERS

=> D SCAN

```
L13 228 ANSWERS   REGISTRY COPYRIGHT 2009 ACS on STN
IN   1,3-Benzenediol, 5-(1-hydroxypentyl)-2-[3-methyl-6-(1-methylethenyl)-2-
    cyclohexen-1-yl]-, [1R-[1a(S*),6β]]- (9CI)
MF   C21 H30 O3
```

Absolute stereochemistry.

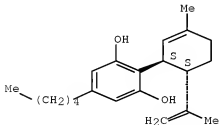


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

```
L13 228 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   1,3-Benzenediol, 2-[(1S,6S)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-
MF   C21 H30 O2
```

Absolute stereochemistry. Rotation (+).



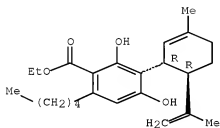
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L13 228 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzoic acid, 2,4-dihydroxy-3-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-6-pentyl-, ethyl ester
 MF C24 H34 O4

Absolute stereochemistry. Rotation (-).

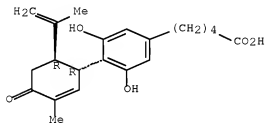


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L13 228 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-methyl-6-(1-methylethenyl)-4-oxo-2-cyclohexen-1-yl]-, (1R-trans)- (9CI)
 MF C21 H26 O5

Absolute stereochemistry.

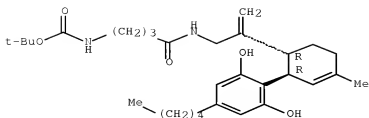


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L13 228 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN Carbamic acid, [4-[[2-[(2-(2,6-dihydroxy-4-pentylphenyl)-4-methyl-3-cyclohexen-1-yl)-2-propenyl]amino]-4-oxobutyl]-, 1,1-dimethylethyl ester, (1R-trans)- (9CI)
 MF C30 H46 N2 O5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FILE STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	186.36	820.40
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.02

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FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Aug 28, 2009 (20090828/UP).

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	820.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.02

FILE 'REGISTRY' ENTERED AT 10:22:42 ON 01 SEP 2009
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STRUCTURE FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8
 DICTIONARY FILE UPDATES: 31 AUG 2009 HIGHEST RN 1178609-15-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

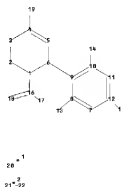
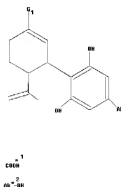
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

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```
chain nodes :
13 14 15 16 17 18 19 20 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-16 4-19 6-9 8-13 10-14 12-15 16-17 16-18 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-19 5-6 8-13 10-14 12-15 21-22
exact bonds :
1-16 6-9 16-17 16-18
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
```

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:CLASS

=> D

L14 HAS NO ANSWERS
L14 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> S L14 SSS SAMPLE

SAMPLE SEARCH INITIATED 10:22:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 197 TO ITERATE

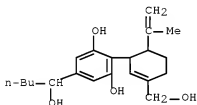
100.0% PROCESSED 197 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3098 TO 4782
PROJECTED ANSWERS: 3 TO 163

L15 3 SEA SSS SAM L14

=> D SCAN

L15 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)-, [1R-[1 α (R*),2 β]]- (9CI)
MF C21 H30 O4

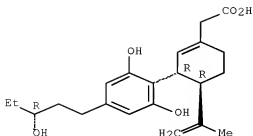


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L15 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (R*),4 β]]- (9CI)
MF C22 H30 O5

Absolute stereochemistry.

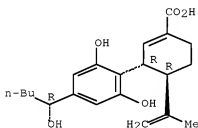


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L15 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(1-
 hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3a(R*),4β]]-
 (9CI)
 MF C21 H28 O5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> 1

1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
 For a list of commands available to you in the current file, enter
 "HELP COMMANDS" at an arrow prompt (=>).

=> S L14 SSS FULL

FULL SEARCH INITIATED 10:23:31 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 3810 TO ITERATE

100.0% PROCESSED 3810 ITERATIONS
 SEARCH TIME: 00.00.01

77 ANSWERS

L16

77 SEA SSS FUL L14

=> D L16 1-77

L16 ANSWER 1 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1101886-13-8 REGISTRY

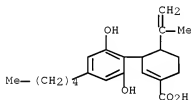
ED Entered STN: 06 Feb 2009

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)- (CA INDEX NAME)

MF C21 H28 O4

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 2 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1101886-10-5 REGISTRY

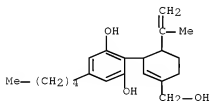
ED Entered STN: 06 Feb 2009

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

MF C21 H30 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

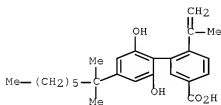
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 3 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1027505-84-5 REGISTRY

ED Entered STN: 12 Jun 2008

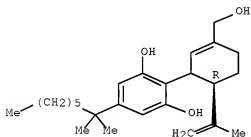
CN INDEX NAME NOT YET ASSIGNED
 MF C25 H32 O4
 SR Other Sources
 Database: ChemSpider (ChemZoo, Inc.)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 ANSWER 4 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 862845-08-7 REGISTRY
 ED Entered STN: 09 Sep 2005
 CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H38 O3
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

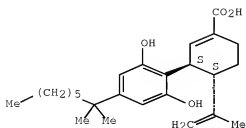


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 5 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 847949-47-7 REGISTRY
 ED Entered STN: 05 Apr 2005
 CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H36 O4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).

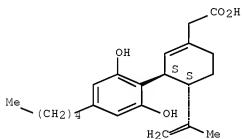


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 6 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 835902-03-9 REGISTRY
ED Entered STN: 23 Feb 2005
CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (+).

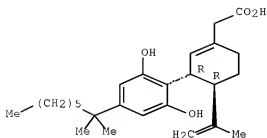


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 7 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 835889-53-7 REGISTRY
ED Entered STN: 23 Feb 2005
CN 1-Cyclohexene-1-acetic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H38 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

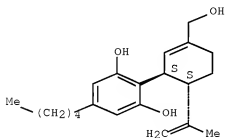
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 8 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 393588-67-5 REGISTRY
ED Entered STN: 19 Feb 2002
CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

OTHER NAMES:

CN (+)-7-Hydroxycannabidiol
FS STEREOSEARCH
MF C21 H30 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).



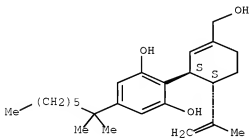
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 9 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 393588-66-4 REGISTRY
ED Entered STN: 19 Feb 2002
CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
FS STEREOSEARCH

MF C25 H38 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).

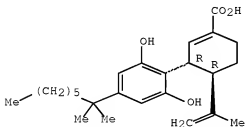


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 10 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 380495-76-1 REGISTRY
ED Entered STN: 04 Jan 2002
CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H36 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, PROUSDDR, SYNTHLINE, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).



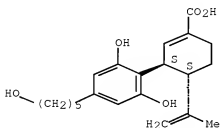
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 11 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 142227-48-3 REGISTRY
ED Entered STN: 03 Jul 1992
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(5-

hydroxypentyl)phenyl]-4-(1-methylethenyl)-, (3S-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C21 H28 O5
 SR CA
 LC STN Files: CA, CAPLUS

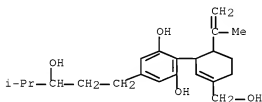
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 12 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 142227-47-2 REGISTRY
 ED Entered STN: 03 Jul 1992
 CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxy-4-methylpentyl)- (CA INDEX NAME)
 MF C22 H32 O4
 SR CA
 LC STN Files: CA, CAPLUS



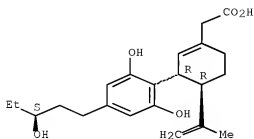
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 13 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 132620-86-1 REGISTRY
 ED Entered STN: 15 Mar 1991
 CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H30 O5

SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

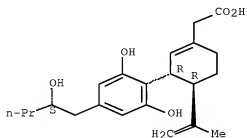


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 14 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132620-85-0 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3a(S*),4β]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



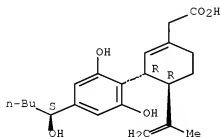
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 15 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132620-84-9 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3a(S*),4β]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
 MF C22 H30 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

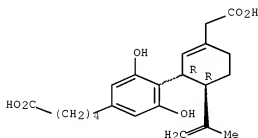


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 16 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 132588-08-0 REGISTRY
 ED Entered STN: 15 Mar 1991
 CN Benzenepentanoic acid, 4-[3-(carboxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H28 O6
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

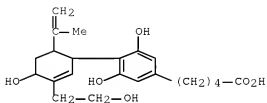


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 17 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 132588-07-9 REGISTRY
 ED Entered STN: 15 Mar 1991
 CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-6-(1-methylethenyl)cyclohex-2-en-1-yl]-

methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
 MF C22 H30 O6
 SR CA
 LC STN Files: CA, CAPLUS

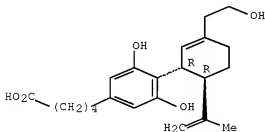


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 18 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 132588-04-6 REGISTRY
 ED Entered STN: 15 Mar 1991
 CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H30 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



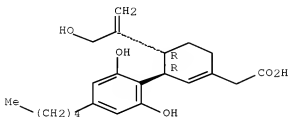
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 19 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 132588-03-5 REGISTRY
 ED Entered STN: 15 Mar 1991
 CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-[1-(hydroxymethyl)ethenyl]-, (3R-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H30 O5

SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

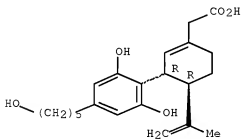


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 20 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132588-02-4 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(5-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

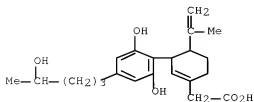


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 21 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132588-01-3 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)
MF C22 H30 O5
SR CA

LC STN Files: CA, CAPLUS

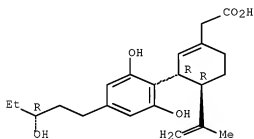


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 22 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132588-00-2 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

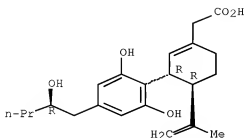


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 23 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-99-6 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

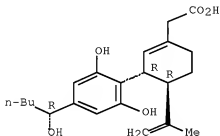


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 24 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-98-5 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypropyl)phenyl]-4-(1-methylethenyl)-, [3R-[3a(R*),4β]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H30 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



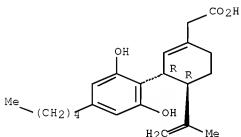
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 25 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-97-4 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R-trans)- (9CI)
FS STEREOSEARCH

MF C22 H30 O4
SR CA
LC STN Files: CA, CAPLUS

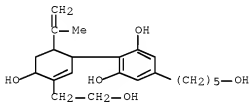
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

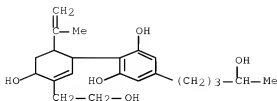
L16 ANSWER 26 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-96-3 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)
MF C22 H32 O5
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

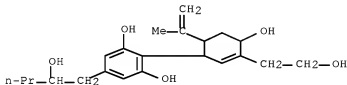
L16 ANSWER 27 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-95-2 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)
MF C22 H32 O5
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

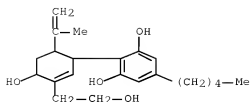
L16 ANSWER 28 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-94-1 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)
MF C22 H32 O5
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

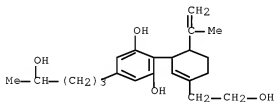
L16 ANSWER 29 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-93-0 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)
MF C22 H32 O4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 30 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-91-8 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)
MF C22 H32 O4
SR CA
LC STN Files: CA, CAPLUS

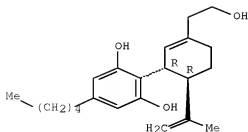


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 31 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 132587-88-3 REGISTRY
ED Entered STN: 15 Mar 1991
CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H32 O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

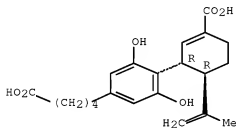


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 32 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-50-6 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzenepentanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H26 O6
SR CA
LC STN Files: CA, CAPLUS

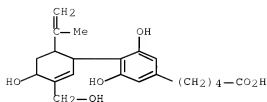
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 33 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-49-3 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
MF C21 H28 O6
SR CA
LC STN Files: CA, CAPLUS

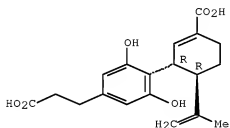


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 34 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-47-1 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzenepropanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H22 O6
SR CA
LC STN Files: CA, CAPLUS

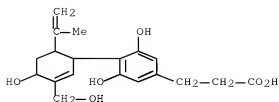
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

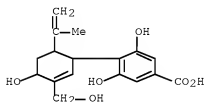
L16 ANSWER 35 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-46-0 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
MF C19 H24 O6
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

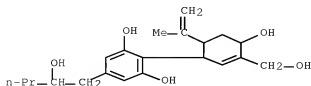
L16 ANSWER 36 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-44-8 REGISTRY
ED Entered STN: 11 Jan 1991
CN Benzoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)
MF C17 H20 O6
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 37 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 131419-41-5 REGISTRY
ED Entered STN: 11 Jan 1991
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O5
SR CA
LC STN Files: CA, CAPLUS

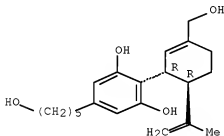


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 38 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130548-70-8 REGISTRY
ED Entered STN: 23 Nov 1990
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H30 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

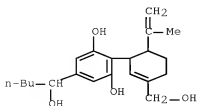
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

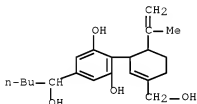
L16 ANSWER 39 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130467-22-0 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)-, [2R-[2 α (S*),3 β]]- (9CI) (CA INDEX NAME)
MF C21 H30 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

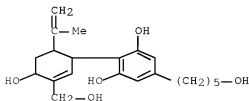
L16 ANSWER 40 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130467-21-9 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)-, [1R-[1 α (R*),2 β]]- (9CI) (CA INDEX NAME)
MF C21 H30 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

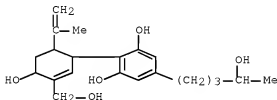
L16 ANSWER 41 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130413-93-3 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O5
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

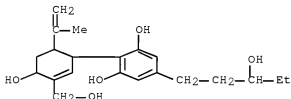
L16 ANSWER 42 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130413-92-2 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O5
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 43 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130413-91-1 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O5
SR CA
LC STN Files: CA, CAPLUS

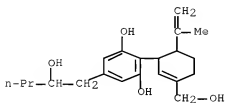


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 44 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 130413-90-0 REGISTRY
ED Entered STN: 16 Nov 1990
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-

yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)
 MF C21 H30 O4
 SR CA
 LC STN Files: CA, CAPLUS

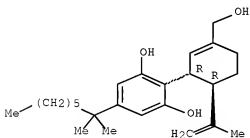


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 45 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 128395-01-7 REGISTRY
 ED Entered STN: 27 Jul 1990
 CN 1,3-Benzenediol, 5-((1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl)- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 1,3-Benzenediol, 5-((1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl)-, (1R-trans)-
 FS STEREOSEARCH
 MF C25 H38 O3
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).

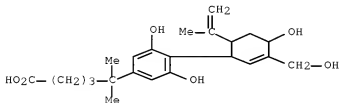


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 46 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 128366-75-6 REGISTRY
 ED Entered STN: 20 Jul 1990
 CN Benzenepentanoic acid, 3,5-dihydroxy-4-((1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl)- (CA INDEX NAME)

methylethenyl)-2-cyclohexen-1-yl]- δ , δ -dimethyl- (CA INDEX
NAME)
MF C23 H32 O6
SR CA
LC STN Files: CA, CAPLUS

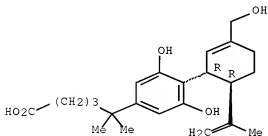


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 47 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 128366-74-5 REGISTRY
ED Entered STN: 20 Jul 1990
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- δ , δ -dimethyl-, (1R-trans)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H32 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 48 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 128366-72-3 REGISTRY
ED Entered STN: 20 Jul 1990
CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-

```

FS      STEREOSEARCH
MF      C22 H30 O5
SR      CA
LC      STN Files:  CA, CAPLUS

```

CC(C)(CC(=O)O)C1=CC=C(C=C1)C2=CC(=C(C=C2)O)C3=C(C=C(C=C3)O)C

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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LN16 ANSWER 49 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RD 127913-41-1 REGISTRY
EN Entered STN: 29 Jun 1990
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-
hydroxyphenyl)phenyl]-4-(1-methylethenyl)-, [3R-[3a(S*),4β]]-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O5
SR CA
LC STN Files: CA, CAPLUS

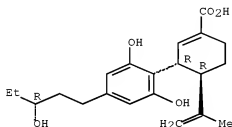
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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 50 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 127913-40-0 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (R*),4 β]]-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C21 H28 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

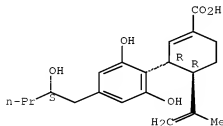


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 51 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 127913-39-7 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (S*),4 β]]-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C21 H28 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

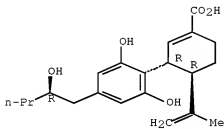


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 52 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 127913-38-6 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (R*),4 β]]-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C21 H28 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

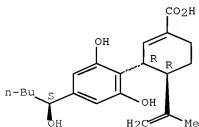


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 53 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 127913-37-5 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (S*),4 β]]-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C21 H28 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

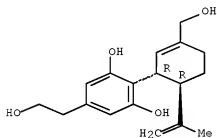


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 54 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 127876-09-9 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1,3-Benzenediol, 5-(2-hydroxyethyl)-2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C18 H24 O4
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

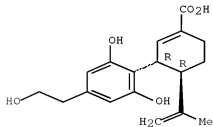


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 55 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 127876-08-8 REGISTRY
 ED Entered STN: 29 Jun 1990
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 DR 129118-71-4
 MF C18 H22 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

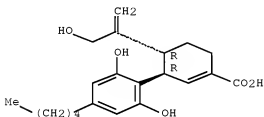


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 56 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 127876-01-1 REGISTRY
ED Entered STN: 29 Jun 1990
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-[1-(hydroxymethyl)ethenyl]-, (3R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

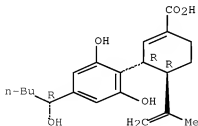


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 57 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 127876-00-0 REGISTRY
ED Entered STN: 29 Jun 1990
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3 α (R*),4 β]]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

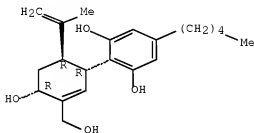


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 58 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 74513-76-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, [1R-(1a,4a,6β)]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

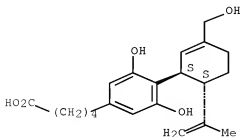


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 59 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 68295-99-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

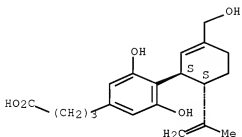


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 60 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 68295-98-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H26 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

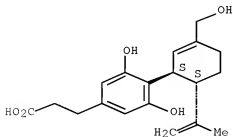


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 61 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 68295-96-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H24 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

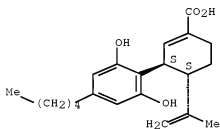


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 62 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 68295-94-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S-trans)-
FS STEREOSEARCH
MF C21 H28 O4
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

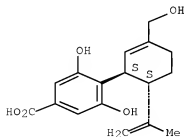


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 63 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 68295-92-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C17 H20 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

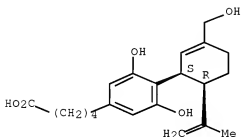


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 64 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 63958-85-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O5
LC STN Files: CA, CAPLUS

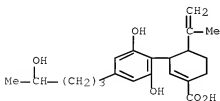
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 65 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 63958-84-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)
MF C21 H28 O5
LC STN Files: CA, CAPLUS

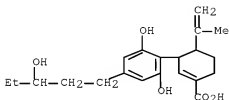


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 66 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 63958-83-8 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)
 MF C21 H28 O5
 LC STN Files: CA, CAPLUS

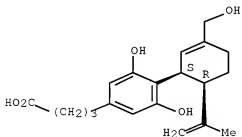


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 67 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 63958-82-7 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Benzenesbutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H26 O5
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

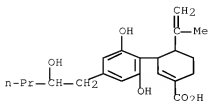


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 68 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 63958-80-5 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)
 MF C21 H28 O5

LC STN Files: CA, CAPLUS

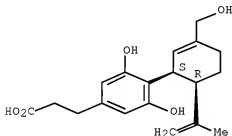


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 69 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 63958-79-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H24 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



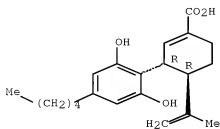
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 70 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 63958-77-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R-trans)-
OTHER NAMES:
CN Cannabidiol-11-oic acid
FS STEREOSEARCH

MF C21 H28 O4
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).

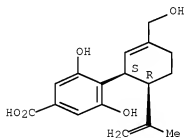


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 71 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 63958-72-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C17 H20 O5
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



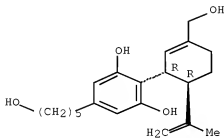
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 72 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 61361-43-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, (1R-trans)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

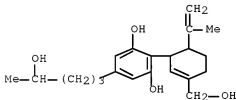
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

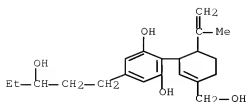
L16 ANSWER 73 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 61361-42-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

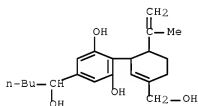
L16 ANSWER 74 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 61361-41-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

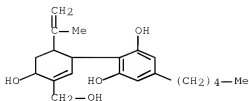
L16 ANSWER 75 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 61361-40-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)- (CA INDEX NAME)
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 76 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN
RN 61361-39-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)
MF C21 H30 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L16 ANSWER 77 OF 77 REGISTRY COPYRIGHT 2009 ACS on STN

RN 50725-17-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)-

OTHER NAMES:

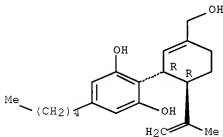
CN 7-Hydroxycannabidiol

FS STEREOSEARCH

MF C21 H30 O3

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS,
NAPRALERT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

23 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
23 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> D HIS

(FILE 'HOME' ENTERED AT 10:00:42 ON 01 SEP 2009)

FILE 'REGISTRY' ENTERED AT 10:01:06 ON 01 SEP 2009
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 1 S L1 SSS FUL
L4 1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:02:40 ON 01 SEP 2009
L5 0 S L4
L6 0 S L3

FILE 'STNGUIDE' ENTERED AT 10:04:28 ON 01 SEP 2009

FILE 'REGISTRY' ENTERED AT 10:08:07 ON 01 SEP 2009
L7 STRUCTURE UPLOADED
L8 0 S L7 SSS SAM
L9 3 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:09:28 ON 01 SEP 2009
L10 11 S L9

FILE 'STNGUIDE' ENTERED AT 10:12:43 ON 01 SEP 2009

FILE 'STNGUIDE' ENTERED AT 10:13:20 ON 01 SEP 2009

FILE 'REGISTRY' ENTERED AT 10:17:39 ON 01 SEP 2009
L11 STRUCTURE UPLOADED
L12 7 S L11 SSS SAMPLE
L13 228 S L11 SSS FULL

— FILE 'STNGUIDE' ENTERED AT 10:18:51 ON 01 SEP 2009

FILE 'REGISTRY' ENTERED AT 10:22:42 ON 01 SEP 2009
L14 STRUCTURE UPLOADED
L15 3 S L14 SSS SAMPLE
L16 77 S L14 SSS FULL

=> FILE CAPLUS		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	352.85	1173.67
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-9.02

FILE 'CAPLUS' ENTERED AT 10:34:29 ON 01 SEP 2009
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 1 Sep 2009 VOL 151 ISS 10
 FILE LAST UPDATED: 31 Aug 2009 (20090831/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> S L16
 L17 36 L16

=> D L17 1-36 IBIB ABS HITSTR

L17 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2008:1007107 CAPLUS Full-text
 DOCUMENT NUMBER: 149:315569
 TITLE: Therapeutic release agents, esters of alkylcarbamic acids, as inhibitors of fatty acid amide hydrolase activity
 INVENTOR(S): Dasse, Olivier; Parrott, Jeff A.; Putman, David; Adam,

PATENT ASSIGNEE(S): Julia
 SOURCE: N.V. Organon, Neth.
 PCT Int. Appl., 250pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008100977	A2	20080821	WO 2008-US53785	20080213
WO 2008100977	A3	20081218		

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2007-889909P P 20070214
 US 2007-948082P P 20070705

OTHER SOURCE(S): MARPAT 149:315569

AB Pharmacol. inhibition of fatty acid amide hydrolase (FAAH) activity leads to increased levels of fatty acid amides. Esters of alkylcarbamic acids are disclosed that are inhibitors of FAAH activity. Comps. disclosed herein inhibit FAAH activity. Described herein are processes for the preparation of esters of alkylcarbamic acid compds., compns. that include them, and methods of use thereof. Thus, to prepare a parenteral pharmaceutical composition for injection, 100 mg of a water-soluble salt of a compound of the invention was dissolved in DMSO and mixed with 10 mL of 0.9% sterile saline; the mixture was incorporated into dosage form unit suitable for administration by injection.

IT 366455-76-1D, derive.

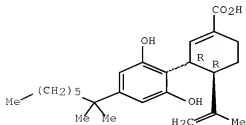
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(therapeutic release agents, esters of alkylcarbamic acids, as inhibitors of fatty acid amide hydrolase activity)

RN 380495-76-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L17 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2006:495679 CAPLUS Full-text
 DOCUMENT NUMBER: 145:167415
 TITLE: Synthesis of Cannabidiols via Alkenylation of Cyclohexenyl Monoacetate
 AUTHOR(S): Kobayashi, Yuichi; Takeuchi, Akira; Wang, Yong-Gang
 CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Yokohama, 226-8501, Japan
 SOURCE: Organic Letters (2006), 8(13), 2699-2702
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:167415

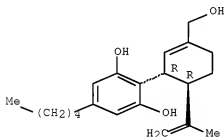
AB Because of the lack of potency binding to the receptors responsible for psychoactivity, cannabidiol has received much attention as a lead compound to develop a nonpsychotropic drug. Herein, we establish a method to access not only cannabidiol but also its analogs. The key reaction is nickel-catalyzed allylation of 2-cyclohexene-1,4-diol monoacetate with a new reagent, (alkenyl)ZnCl/TMEDA, which gives a SN2-type product with 94% regioselectivity in good yield.

IT 50725-17-2P, 7-Hydroxycannabidiol
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (synthesis of cannabidiols via regioselective alkenylation of cyclohexenyl monoacetate)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
 REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:463190 CAPLUS Full-text
 DOCUMENT NUMBER: 143:222241
 TITLE: Evidence that (-)-7-hydroxy-4'-dimethylheptyl-cannabidiol activates a non-CB1, non-CB2, non-TRPV1 target in the mouse via deferens
 AUTHOR(S): Pertwee, Roger G.; Thomas, Adele; Stevenson, Lesley A.; Maor, Yehoshua; Mechoulam, Raphael
 CORPORATE SOURCE: School of Medical Sciences, Institute of Medical Sciences, University of Aberdeen, Aberdeen,

SOURCE: Foresterhill, AB25 2ZD, UK
Neuropharmacology (2005), 48(8), 1139-1146
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Previous expts. showed that R-(+)-WIN55212-induced inhibition of elec.-evoked contractions of mouse vasa deferentia could be antagonized by cannabidiol in a manner that appeared to be competitive but not to involve direct competition for established cannabinoid receptors. We have now discovered that (-)-7-hydroxy-4'-dimethylheptyl-cannabidiol (7-OH-DMH-CBD) inhibits elec.-evoked contractions of the vas deferens (EC50 = 13.3 nM). This it appeared to do by acting on prejunctional neurons as 100 nM 7-OH-DMH-CBD did not attenuate contractile responses to phenylephrine or β , γ -methylene-ATP. Although 7-OH-DMH-CBD was antagonized by SR141716A, it was less susceptible to antagonism by this CB1 receptor antagonist than R-(+)-WIN55212. 7-OH-DMH-CBD was also antagonized by cannabidiol (1 μ M; apparent KB = 222.2 nM) but not by the CB2 receptor antagonist, SR144528 (32 nM), or by naloxone (300 nM), ruthenium red (1 μ M) or capsazepine (10 μ M). Yohimbine (100 nM) enhanced the ability of 7-OH-DMH-CBD to inhibit elec.-evoked contractions. R-(+)-WIN55212 was also potentiated by 100 nM yohimbine, possibly reflecting ongoing sequestration of Gi/o proteins from CB1 receptors by α 2-adrenoceptors. Our results suggest that 7-OH-DMH-CBD may activate a neuronal target in the vas deferens that is not a CB1, CB2, TRPV1, opioid or α 2-adrenergic receptor but do not exclude the possibility that it also activates CB1 receptors.

IT 862845-08-7

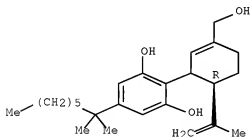
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(evidence that (-)-7-hydroxy-4'-dimethylheptyl-cannabidiol activates a non-CB1, non-CB2, non-TRPV1 target in mouse vas deferens)

RN 862845-08-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2005:463188 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:206227

TITLE: Peripheral, but not central effects of cannabidiol derivatives: Mediation by CB1 and unidentified receptors

AUTHOR(S): Fride, Ester; Ponde, Datta; Breuer, Aviva; Hanus, Lumir
 CORPORATE SOURCE: Department of Behavioral Sciences, College of Judea and Samaria, Ariel, 44837, Israel
 SOURCE: Neuropharmacology (2005), 48(8), 1117-1129
 CODEN: NEPHBW; ISSN: 0028-3908
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Delta-9 tetrahydrocannabinol (Δ^9 -THC) and (-)-cannabidiol ((-)-CBD) are major constituents of the Cannabis sativa plant with different pharmacol. profiles: Δ^9 -THC activates cannabinoid CB1 and CB2 receptors and induces psychoactive and peripheral effects. (-)-CBD possesses no, or very weak affinity for these receptors. The authors tested a series of (+)- and (-)-CBD derivs. for central and peripheral effects in mice. None of the (-)-CBD derivs. were centrally active, yet most inhibited intestinal motility. Of the five (+)-CBD derivs., all with CB1 receptor affinity, only (+)-7-OH-CBD-DMH (DMH = 1,1-dimethylheptyl), acted centrally, while all five arrested defecation. The effects of (+)-CBD-DMH and (+)-7-OH-CBD-DMH were inhibited by the CB1 receptor antagonist SR141716. The CB2 receptor antagonist SR144528, and the vanilloid TRPV1 receptor antagonist capsazepine, had no influence. Further, the (-)-CBD derivs. (-)-7-COOH-CBD and (-)-7-COOH-CBD-DMH, displayed anti-inflammatory activity. The authors suggest that (+)-CBD analogs have mixed agonist/antagonist activity in the brain. Second, (-)-CBD analogs which are devoid of cannabinoid receptor affinity but which inhibit intestinal motility, suggest the existence of a non-CB1, non-CB2 receptor. Therefore, such analogs should be further developed as antidiarrheal and/or anti-inflammatory drugs. The authors propose to study the therapeutic potential of (-)- and (+)-CBD derivs. for complex conditions such as inflammatory bowel disease and cystic fibrosis.

IT 50725-17-2 63958-77-0 68295-94-3
 128395-01-7 380495-76-1 393588-66-4
 393588-67-5 847949-47-7

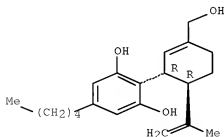
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peripheral, but not central effects of cannabidiol derivs. and mediation by CB1 and unidentified receptors)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

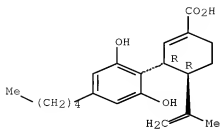
Absolute stereochemistry. Rotation (-).



RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

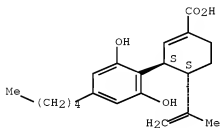
Absolute stereochemistry. Rotation (-).



RN 68295-94-3 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

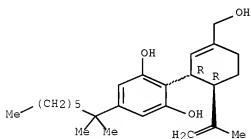
Absolute stereochemistry.



RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

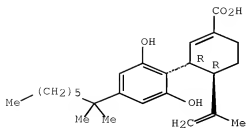
Absolute stereochemistry. Rotation (-).



RN 380495-76-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

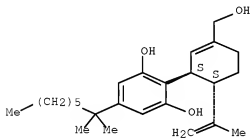
Absolute stereochemistry. Rotation (-).



RN 393588-66-4 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

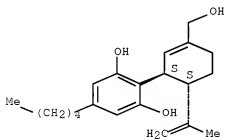
Absolute stereochemistry. Rotation (+).



RN 393588-67-5 CAPLUS

CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

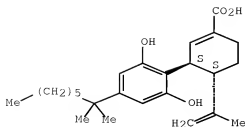
Absolute stereochemistry. Rotation (+).



RN 847949-47-7 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2005:238931 CAPLUS Full-text

DOCUMENT NUMBER: 142:316978

TITLE: Preparation of (+)-cannabidiol derivatives for use in pharmaceutical compositions as immune system modulators, analgesics and anti-inflammatory agents

INVENTOR(S): Mechoulam, Raphael; Fride, Ester

PATENT ASSIGNEE(S): Yissum Research Development Company of the Hebrew University of Jerusalem, Israel; Ariel Ltd.

SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2

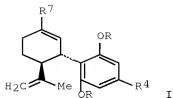
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023741	A2	20050317	WO 2004-IL810	20040908
WO 2005023741	A3	20050421		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070082954	A1	20070412	US 2006-570737	20060928
PRIORITY APPLN. INFO.:			IL 2003-157849	A 20030910
			WO 2004-IL810	W 20040908
OTHER SOURCE(S):		CASREACT 142:316978; MARPAT 142:316978		
GI				



AB (+)-Cannabidiol derivs., such as I [R = H; R4 = (CH2)4Me, CMe2(CH2)5Me; R7 = CH2OH, CO2H], were prepared for therapeutic use as agents which have selective activity in the peripheral and not in the central nervous system. These (+)-cannabidiols are claimed for use as analgesics, immunomodulators and anti-inflammatory agents useful for the treatment of diseases and conditions, such as inflammatory bowel disease, diarrhea and inflammatory pain. Thus, (+)-cannabidiol derivative I [R = H, R4 = (CH2)4Me, R7 = CH2OH] was prepared via a multistep synthesis starting from (+)-cannabidiol I [R = H, R4 = (CH2)4Me, R7 = Me]. The prepared (+)-cannabidiol derivs. were screened for a variety of pharmacol. activities, such as CB1 and CB2 type cannabinoid receptor binding, analgesic activity and inhibition of intestinal motility.

IT 68295-24-3P 393588-66-4P 393588-67-5P
847949-47-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

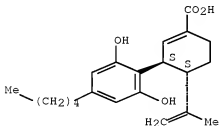
(preparation of (+)-cannabidiol derivs. for use in pharmaceutical comps.

as immune system modulators, analgesics and anti-inflammatory agents)

RN 68295-94-3 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

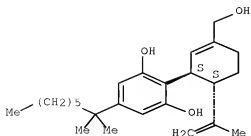
Absolute stereochemistry.



RN 393588-66-4 CAPLUS

CN 1,3-Benzenediol, 5-[(1,1-dimethylheptyl)-2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]]- (CA INDEX NAME)

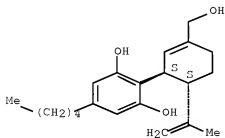
Absolute stereochemistry. Rotation (+).



RN 393588-67-5 CAPLUS

CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

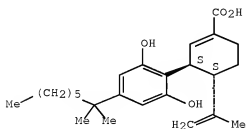
Absolute stereochemistry. Rotation (+).



RN 847949-47-7 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:199003 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:447306

TITLE: Enantiomeric cannabidiol derivatives: synthesis and binding to cannabinoid receptors

AUTHOR(S): Hanus, Lumir O.; Tchilibon, Susanna; Ponde, Datta E.; Breuer, Aviva; Friede, Ester; Mechoulam, Raphael

CORPORATE SOURCE: Department of Medicinal Chemistry and Natural

Products, School of Pharmacy, Medical Faculty, The Hebrew University of Jerusalem, Jerusalem, 91120, Israel

SOURCE: Organic & Biomolecular Chemistry (2005), 3(6), 1116-1123

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:447306

AB (-)-Cannabidiol (CBD) is a major, non psychotropic constituent of cannabis. It has been shown to cause numerous physiol. effects of therapeutic importance. We have reported that CBD derivs. in both enantiomeric series are of pharmaceutical interest. Here we describe the syntheses of the major CBD metabolites, (-)-7-hydroxy-CBD and (-)-CBD-7-oic acid and their dimethylheptyl (DMH) homologs, as well as of the corresponding compds. in the enantiomeric (+)-CBD series. The starting materials were the resp. CBD enantiomers and their DMH homologs. The binding of these compds. to the CB1 and CB2 cannabinoid receptors are compared. Surprisingly, contrary to the compds. in the (-) series, which do not bind to the receptors, most of the derivs. in the (+) series bind to the CB1 receptor in the low nanomole range. Some of these compds. also bind weakly to the CB2 receptor.

IT 50725-17-2P 63958-77-0P 66295-94-3P

380495-76-1P 393586-67-5P 847949-47-7P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

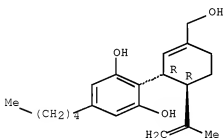
BIOL (Biological study); PREP (Preparation)

(preparation of enantiomeric cannabidiol derivs. and their binding to cannabinoid receptors)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

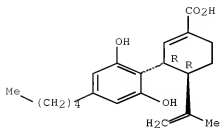
Absolute stereochemistry. Rotation (-).



RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

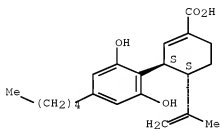
Absolute stereochemistry. Rotation (-).



RN 68295-94-3 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

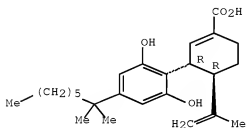
Absolute stereochemistry.



RN 380495-76-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

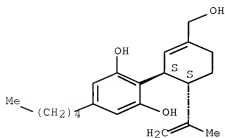
Absolute stereochemistry. Rotation (-).



RN 393588-67-5 CAPLUS

CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

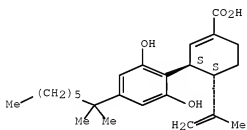
Absolute stereochemistry. Rotation (+).



RN 847949-47-7 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



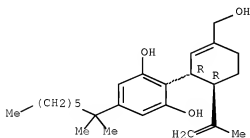
IT 128395-01-7P 393588-66-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of enantiomeric cannabidiol derivs. and their binding to cannabinoid receptors)

RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

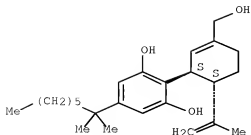
Absolute stereochemistry. Rotation (-).



RN 393588-66-4 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS
RECORD (10 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2004:1054001 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:191011

TITLE: (+)-Cannabidiol analogues which bind cannabinoid

receptors but exert peripheral activity only

AUTHOR(S): Fride, Ester; Feigin, Cfir; Ponde, Datta E.; Breuer,
Aviva; Hanus, Lumir; Arshavsky, Nina; Mechoulam,
Raphael

CORPORATE SOURCE: Department of Behavioral Sciences, College of Judea
and Samaria, Ariel, 44837, Israel

SOURCE: European Journal of Pharmacology (2004), 506(2),
179-188

CODEN: EJPHAZ; ISSN: 0014-2999

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Δ9-Tetrahydrocannabinol (Δ9-THC) and (-)-cannabidiol are major constituents of the Cannabis sativa plant with different pharmacol. profiles: (-)-Δ9-tetrahydrocannabinol, but not (-)-cannabidiol, activates cannabinoid CB1 and CB2 receptors and induces psychoactive and peripheral effects. We have tested a series of (+)-cannabidiol derivs., namely, (+)-cannabidiol-DMH (DMH-1,1-dimethylheptyl-), (+)-7-OH-cannabidiol-DMH, (+)-7-OH-cannabidiol, (+)-7-COOH-cannabidiol and (+)-7-COOH-cannabidiol-DMH, for central and peripheral (intestinal, antiinflammatory and peripheral pain) effects in mice. Although all (+)-cannabidiols bind to cannabinoid CB1 and CB2 receptors, only (+)-7-OH-cannabidiol-DMH was centrally active, while all (+)-cannabidiol analogs completely arrested defecation. The effects of (+)-cannabidiol-DMH and (+)-7-OH-cannabidiol-DMH were partially antagonized by the cannabinoid CB1 receptor antagonist SR141716, but not by the cannabinoid CB2 receptor antagonist SR144528, and had no effect on CB-/-1 receptor knockout mice. (+)-Cannabidiol-DMH inhibited the peripheral pain response and arachidonic-acid-induced inflammation of the ear. We conclude that centrally inactive (+)-cannabidiol analogs should be further developed as antidiarrheal, antiinflammatory and analgesic drugs for gastrointestinal and other peripheral conditions.

IT 393588-66-4 393588-67-5, (+)-7-Hydroxycannabinol

835889-53-7 835892-03-9

RL: PAC (Pharmacological activity); BIOL (Biological study)

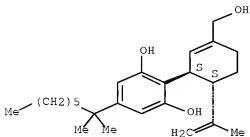
((+)-cannabidiol analogs which bind cannabinoid receptors but exert peripheral activity only)

RN 393588-66-4 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[1S,6S]-3-(hydroxymethyl)-6-(1-

methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

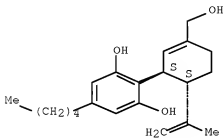
Absolute stereochemistry. Rotation (+).



RN 393588-67-5 CAPLUS

CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

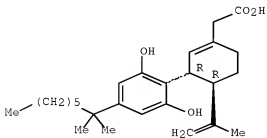
Absolute stereochemistry. Rotation (+).



RN 835889-53-7 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

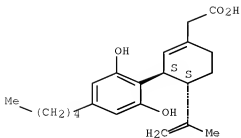
Absolute stereochemistry. Rotation (+).



RN 835902-03-9 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS
RECORD (23 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2004:64549 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:66371

TITLE: Comprehensive profiling of drugs of abuse in
biological fluids by stir-bar sorptive
extraction-thermal desorption-capillary gas
chromatography-mass spectrometry

AUTHOR(S): Tienpont, Bart; David, Frank; Stopforth, Adriana;
Sandra, Pat

CORPORATE SOURCE: Research Institute for Chromatography, Kortrijk, Belg.

SOURCE: LC-GC Europe (2003), 16(12a), 5-13

CODEN: LCGCB4; ISSN: 1471-6577

PUBLISHER: LC-GC Europe

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This article presents a comprehensive approach to capillary GC-MS data handling and mapping of specific target analytes, illustrated with the detection of drugs of abuse in biol. fluids. The word "comprehensive" is used here in sensu stricto, i.e., including everything one wants to detect. Enrichment of the target solutes is performed by stir-bar sorptive extraction (SBSE) followed by thermal desorption-capillary gas chromatog.-mass spectrometry (TD-CGC-MS) anal. The high sensitivity that can be reached with the SBSE-TD-CGC-MS technique allows the use of MS in scan mode. The GC-MS data are plotted in a contour plot with locked retention times in the x-axis and ion traces in the y-axis. Target solutes are identified by a spot in specific positions in the plot and the color of the spots is related to peak abundances. Semi-quant. information can be readily obtained from the contour plots while precise quantification requires conventional calibration procedures. The graphical representation of CGC-MS data provides an easy way for non-skilled personnel in forensic and medical labs. to confirm pos. drugs-of-abuse samples.

IT 50725-17-2, 7-Hydroxycannabidiol

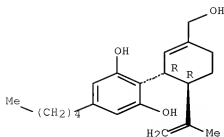
RL: ADV (Adverse effect, including toxicity); ANT (Analyte); BSU
(Biological study, unclassified); ANST (Analytical study); BIOL
(Biological study)

(profiling of drugs of abuse in biol. fluids by stir-bar sorptive
extraction-thermal desorption-capillary gas chromatog.-mass spectrometry)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2009 ACS ON STN
ACCESSION NUMBER: 2001:923605 CAPLUS Full-text
DOCUMENT NUMBER: 136:42873
TITLE: Pharmaceutical compositions comprising cannabidiol
derivatives
INVENTOR(S): Mechoulam, Raphael; Tchilibon, Susana; Frider, Ester;
Hanus, Lumir; Breuer, Aviva; Gallily, Ruth
PATENT ASSIGNEE(S): Yissum Research Development Company of the Hebrew
University of Jerusalem, Israel
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095899	A2	20011220	WO 2001-IL537	20010612
WO 2001095899	A3	20020808		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
IL 136839	A	20061210	IL 2000-136839	20000616
CA 2411831	A1	20011220	CA 2001-2411831	20010612
EP 1289517	A2	20030312	EP 2001-940973	20010612
EP 1289517	B1	20051116		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004503498	T	20040205	JP 2002-510078	20010612
AU 2001274459	B2	20050707	AU 2001-274459	20010612
AT 309798	T	20051215	AT 2001-940973	20010612
ES 2254432	T3	20060616	ES 2001-940973	20010612
IN 2002DN01197	A	20080926	IN 2002-DN1197	20021205

IN 2002DN01198	A	20080926	IN 2002-DN1198	20021205
US 20030166727	A1	20030904	US 2003-311554	20030130
PRIORITY APPLN. INFO.:			IL 2000-136839	A 20000616
			WO 2001-IL537	W 20010612

OTHER SOURCE(S): MARPAT 136;42873

AB Pharmaceutical compns. of the present invention comprise cannabidiol derivs. as antiinflammatory agents having analgesic, antianxiety, anticonvulsive, neuroprotective, antipsychotic and anticancer activity. A process for the preparation of cannabidiol derivs. is also described. Compns. of cannabidiol derivs. are selected from a tablet, a capsule, a granule, and a suspension in a solution. For example, 7-hydroxy-cannabidiol and 7-hydroxy-cannabidiol-1',1'-dimethylheptyl derivative showed anti-inflammatory activity. 7-Hydroxy-cannabidiol in doses of 10 µg/kg i.p. suppressed serum tumor necrosis factor α in mice (30%). 7-Hydroxy-cannabidiol and 7-hydroxy-cannabidiol-1',1'-dimethylheptyl derivative also inhibited NO generation by murine macrophages (up to 90%). Generation of oxygen radicals intermediate (ROI) by macrophages was almost totally inhibited (up to 95%) when cells were incubated with cannabidiol-7-oic acid and cannabidiol-1',1'-dimethylheptyl-7-oic acid. Cannabidiol and other compds., such as cannabidiol-1',1'-dimethylheptyl-7-oic acid caused high rate of programmed cell death (apoptosis) in human HL-60 promyelocytic leukemia cells. The apoptosis was cannabidiol dose dependent (0.1-8 µg/mL). Moreover, a marked synergism reaching 85% of apoptosis was seen when HL-60 cells were irradiated by γ-ray (800 rad) and treated with cannabidiol and/or other compds. of this invention.

IT 50725-17-2F 128395-01-7F

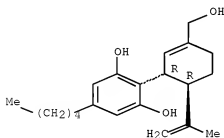
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation and compns. of cannabidiol derivs. as anti-inflammatory agents with analgesic, antianxiety, anticonvulsive, neuroprotective, antipsychotic and anticancer activity)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

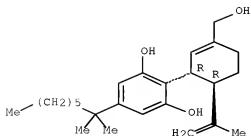
Absolute stereochemistry. Rotation (-).



RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 63958-77-0F 380495-76-1F

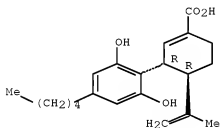
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and comps. of cannabidiol derivs. as anti-inflammatory agents with analgesic, antianxiety, anticonvulsive, neuroprotective, antipsychotic and anticancer activity)

RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

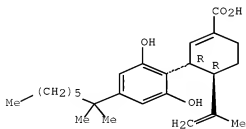
Absolute stereochemistry. Rotation (-).



RN 380495-76-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2001:834237 CAPLUS Full-text

DOCUMENT NUMBER: 136:128587

TITLE: Molecular targets for cannabidiol and its synthetic analogues: effect on vanilloid VR1 receptors and on the cellular uptake and enzymatic hydrolysis of anandamide

AUTHOR(S): Bisogno, Tiziana; Hanus, Lumir; De Petrocellis, Luciano; Tchilibon, Susanna; Ponde, Datta E.; Brandi, Ines; Moriello, Aniello Schiano; Davis, John B.; Mechoulam, Raphael; Di Marzo, Vincenzo

CORPORATE SOURCE: Endocannabinoid Research Group, Istituto per la Chimica di Molecole di Interesse Biologico, Consiglio Nazionale delle Ricerche, Naples, 80078, Italy

SOURCE: British Journal of Pharmacology (2001), 134(4), 845-852

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (-)-Cannabidiol (CBD) is a non-psychotropic component of Cannabis with possible therapeutic use as an anti-inflammatory drug. Little is known on the possible mol. targets of this compound. We investigated whether CBD and some of its derivs. interact with vanilloid receptor type 1 (VR1), the receptor for capsaicin, or with proteins that inactivate the endogenous cannabinoid, anandamide (AEA). CBD and its enantiomer, (+)-CBD, together with seven analogs, obtained by exchanging the C-7 Me group of CBD with a hydroxy-Me or a carboxyl function and/or the C-5' pentyl group with a di-methyl-heptyl (DMH) group, were tested on: (a) VR1-mediated increase in cytosolic Ca^{2+} concns. in cells over-expressing human VR1; (b) [^{14}C]-AEA uptake by RBL-2H3 cells, which is facilitated by a selective membrane transporter; and (c) [^{14}C]-AEA hydrolysis by rat brain membranes, which is catalyzed by the fatty acid amide hydrolase. Both CBD and (+)-CBD, but not the other analogs, stimulated VR1 with EC_{50} =3.2-3.5 μM , and with a maximal effect similar in efficacy to that of capsaicin, i.e. 67-70% of the effect obtained with ionomycin (4 μM). CBD (10 μM) desensitized VR1 to the action of capsaicin. The effects of maximal doses of the two compds. were not additive. (+)-5'-DMH-CBD and (+)-7-hydroxy-5'-DMH-CBD inhibited [^{14}C]-AEA uptake (IC_{50} =10.0 and 7.0 μM); the (-)-enantiomers were slightly less active (IC_{50} =14.0 and 12.5 μM). CBD and (+)-CBD were also active (IC_{50} =22.0 and 17.0 μM). CBD (IC_{50} =27.5 μM), (+)-CBD (IC_{50} =63.5 μM) and (-)-7-hydroxy-CBD (IC_{50} =34 μM), but not the other analogs (IC_{50} >100 μM), weakly inhibited [^{14}C]-AEA hydrolysis. Only the (+)-isomers exhibited high affinity for CB1 and/or CB2 cannabinoid receptors. These findings suggest that VR1 receptors, or increased levels of endogenous AEA, might mediate some of the pharmacol. effects of CBD and its analogs. In view of the facile high yield synthesis, and the weak affinity for CB1 and CB2 receptors, (-)-5'-DMH-CBD represents a valuable candidate for further investigation as inhibitor of AEA uptake and a possible new therapeutic agent.

IT 50725-17-2 128395-01-7 380495-76-1
393588-66-4 393588-67-5

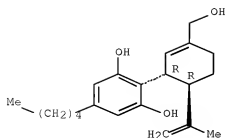
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
BIOL (Biological study)

(effect of cannabidiol and synthetic analogs on vanilloid VR1 receptors and on cellular uptake and enzymic hydrolysis of anandamide)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

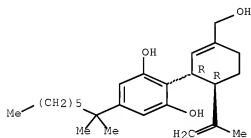
Absolute stereochemistry. Rotation (-).



RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

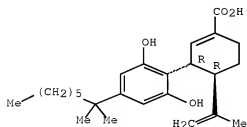
Absolute stereochemistry. Rotation (-).



RN 380495-76-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[4-(1,1-dimethylheptyl)-2,6-dihydroxyphenyl]-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

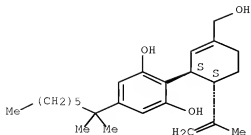
Absolute stereochemistry. Rotation (-).



RN 393588-66-4 CAPLUS

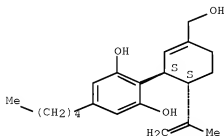
CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



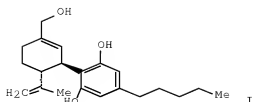
RN 393588-67-5 CAPLUS
 CN 1,3-Benzenediol, 2-[(1S,6S)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 136 THERE ARE 136 CAPLUS RECORDS THAT CITE THIS RECORD (136 CITINGS)
 REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

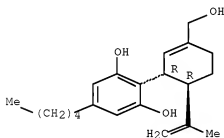
L17 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:653207 CAPLUS Full-text
 DOCUMENT NUMBER: 133:350353
 TITLE: Synthesis of a Primary Metabolite of Cannabidiol
 AUTHOR(S): Tchilibon, Susanna; Mechoulam, Raphael
 CORPORATE SOURCE: Department of Medicinal Chemistry and Natural Products
 School of Pharmacy, Hebrew University Medical Faculty,
 Jerusalem, 91120, Israel
 SOURCE: Organic Letters (2000), 2(21), 3301-3303
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:350353
 GI



AB Cannabidiol is the major non-psychotropic, neutral constituent in most cannabis preps. It is devoid of the psychoactive properties typical of cannabis; however, it produces numerous, potentially therapeutic pharmacol. effects, some of which may be due to its metabolites. The authors report now the first total synthesis of 7-hydroxycannabidiol I, a primary metabolite of cannabidiol, in an eight-step procedure.

IT 50725-17-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of a primary metabolite of cannabidiol)
 RN 50725-17-2 CAPLUS
 CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
 REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1999:690951 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 131:307105
 TITLE: Cannabinoids as antioxidants and neuroprotectants
 INVENTOR(S): Hampson, Aidan J.; Axelrod, Julius; Grimaldi, Maurizio
 PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
 SOURCE: PCT Int. Appl., 48 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9953917	A1	19991028	WO 1999-US8769	19990421

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
 DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
 JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,
 MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
 TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
 ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2329626	A1	19991028	CA 1999-2329626	19990421
AU 9938646	A	19991108	AU 1999-38646	19990421
AU 766988	B2	20031030		
EP 1071419	A1	20010131	EP 1999-921427	19990421
EP 1071419	B1	20070725		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, FI, CY

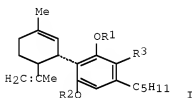
JP 2002512188	T	20020423	JP 2000-544322	19990421
AT 367809	T	20070815	AT 1999-921427	19990421
US 6630507	B1	20031007	US 2001-674028	20010202

PRIORITY APPLN. INFO.:

US 1998-82589P	P	19980421
US 1998-95993P	P	19980810
WO 1999-US8769	W	19990421

OTHER SOURCE(S): MARPAT 131:307105

GI



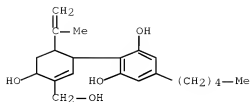
AB Cannabinoids have been found to have antioxidant properties, unrelated to NMDA receptor antagonism. This new found property makes the cannabinoids useful in the treatment and prophylaxis of a wide variety of oxidation-associated diseases, such as ischemic, age-related, inflammatory and autoimmune diseases. The cannabinoids are found to have particular application as neuroprotectants, for example in limiting neurol. damage following ischemic insults, such as stroke and trauma, or in the treatment of neurodegenerative diseases, such as Alzheimer's disease, Parkinson's disease and HIV dementia. Nonpsychoactive cannabinoids, such as cannabidiol, are particularly advantageous to use because they avoid toxicity that is encountered with psychoactive cannabinoids at high doses useful in the method of the present invention. A particular disclosed class of cannabinoids useful as neuroprotective antioxidants is I (R1, R2, R3 = H, CH3, and COCH3). Cannabidiol protected neurons against reactive oxygen species toxicity in a dose related manner, with an EC50 of about 6 μ M.

IT 61361-39-5 61361-41-9 61361-42-0
 1101886-10-5 1101886-13-6
 RL: PRPH (Prophetic)

(Cannabinoids as antioxidants and neuroprotectants)

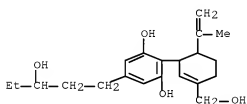
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



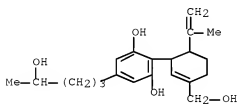
RN 61361-41-9 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)



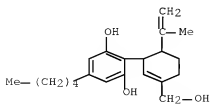
RN 61361-42-0 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 1101886-10-5 CAPLUS

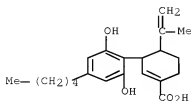
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



RN 1101886-13-8 CAPLUS

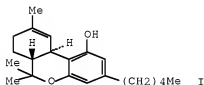
CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-

methylethenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1993:75078 CAPLUS Full-text
 DOCUMENT NUMBER: 118:75078
 ORIGINAL REFERENCE NO.: 118:13051a,13054a
 TITLE: Comparative in vitro metabolism of the cannabinoids
 AUTHOR(S): Harvey, D. J.; Brown, N. K.
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK
 SOURCE: Pharmacology, Biochemistry and Behavior (1991), 40(3), 533-40
 CODEN: PBBHAU; ISSN: 0091-3057
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The metab. of delta-9-tetrahydrocannabinol (delta-9-THC, I), delta-8-THC, delta-11-THC, cannabidiol (CBD), cannabinol (CBN), cannabichromene (CBC), cannabigerol (CBG), and the equatorial-isomer of hexahydrocannabinol (HHC) was studied in liver microsomal preps. from rats, mice, guinea pigs, rabbits, hamsters, gerbils, and a cat. Identification of metabolites was by GC/MS and quantification by gas chromatog. Major metabolites were monohydroxylated compds. but the pattern of hydroxylation varied considerably between the species, reflecting the variable nature of the cytochrome P 450 mixed-function oxidases. Although the primary carbon allylic to the endocyclic double bond of tricyclic cannabinoids was usually the major site of attach, the 4' (side-chain, omega-1 position) and the terpene ring were usually favored in the cat and hamster, resp. The guinea pig generally produced more metabolites hydroxylated in the side-chain (all positions) than did the other species. The results from HHC were very similar to those from THC, namely hydroxylation at C-11 in most species, and the production of high concns. of 8- α -hydroxy-HHC in the mouse and 8- β -hydroxy-HHC in the hamster. As this mol. lacks the

double bond of the THC's and the allylic nature of C-11 and C-8, the orientation of the mol. to the active site of the cytochrome P 450 mixed-function oxidase rather than the reactivity of the C-H bond may govern the position of hydroxylation.

IT 50725-17-2

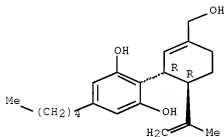
RL: FORM (Formation, nonpreparative)

(formation of, as cannabinoid metabolite, by liver microsomes, species differences in)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L17 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:439733 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 117:39733

ORIGINAL REFERENCE NO.: 117:6819a,6822a

TITLE: Metabolism of cannabidiol by the rat

AUTHOR(S): Samara, E.; Bialer, M.; Harvey, D. J.

CORPORATE SOURCE: Univ. Dep. Pharmacol., Oxford, UK

SOURCE: European Journal of Drug Metabolism and

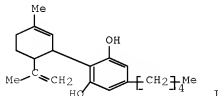
Pharmacokinetics (1991), 16(4), 305-313

CODEN: EJDPD2; ISSN: 0398-7639

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Metabolites of cannabidiol (CBD) (I) excreted into the bile and perfusion fluid were examined in a rat liver perfusion preparation. Metabolites were extracted with Et acetate and identified by GC/mass spectrometry (MS) as TMS derivs. Four mono- and five dihydroxy metabolites were identified with major

sites of metabolic attack being at C-7 and C-4''. A hydroxy-ketone was detected but not fully identified. All biliary metabolites were conjugated with glucuronic acid. Urinary metabolites were studied in rats with samples taken at times to 25 h after drug administration. Unmetabolized CBD and 13 metabolites were identified by GC/MS. Major metabolites were acids with beta-oxidation being a prominent pathway. The 6- and 7-hydroxy derivs. of 4'', 5''-bis,nor-CBD-3''-oic acid were the most abundant compds. but substantial concns. of the di-acids, CBD-5'',7-dioic acid and 4'',5''-bis,nor-CBD-3'',7-dioic acid were present. Concns. of the more highly oxidized metabolites increased with time.

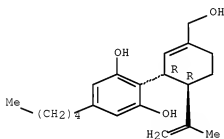
IT 50725-17-2 61361-39-5 61361-42-0
 61361-43-1 63958-72-5 63958-73-2
 63958-84-9 127876-06-8 130413-92-2
 130413-93-3 131419-46-0 131419-47-1
 131419-50-6 142227-47-2 142227-48-3

RL: BIOL (Biological study)
 (as cannabidiol metabolite)

RN 50725-17-2 CAPLUS

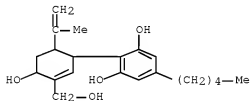
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



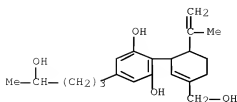
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

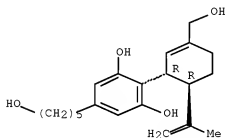
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 61361-43-1 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, (1R-trans)- (9CI) (CA INDEX NAME)

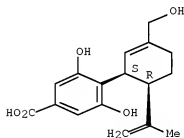
Absolute stereochemistry.



RN 63958-72-5 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

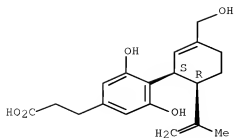
Absolute stereochemistry.



RN 63958-79-2 CAPLUS

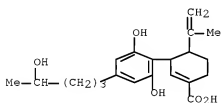
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 63958-84-9 CAPLUS

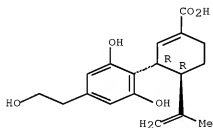
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 127876-08-8 CAPLUS

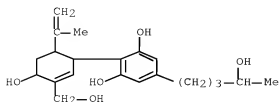
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



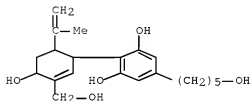
RN 130413-92-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



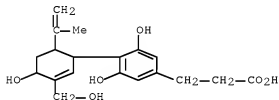
RN 130413-93-3 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)



RN 131419-46-0 CAPLUS

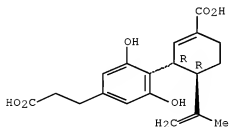
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-47-1 CAPLUS

CN Benzenepropanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

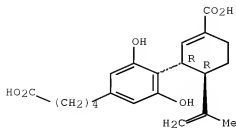
Absolute stereochemistry.



RN 131419-50-6 CAPLUS

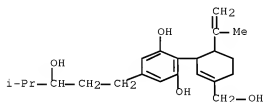
CN Benzenepentanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 142227-47-2 CAPLUS

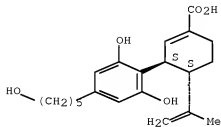
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxy-4-methylpentyl)- (CA INDEX NAME)



RN 142227-48-3 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(5-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:187416 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 116:187416

ORIGINAL REFERENCE NO.: 116:31487a,31490a

TITLE: Comparative metabolism of cannabidiol in dog, rat and man

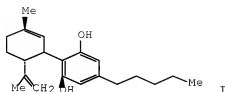
AUTHOR(S): Harvey, D. J.; Samara, E.; Mechoulam, R.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK

SOURCE: Pharmacology, Biochemistry and Behavior (1991), 40(3), 523-32

CODEN: PBBHAU; ISSN: 0091-3057

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Urinary metabolites of cannabidiol (CBD, I) were extd. from human, dog, and rat urine, concentrated by chromatog. on Sephadex LH-20, and identified by GC/MS. Over 50 metabolites were identified, with considerable species variation. CBD was excreted in substantial concentration in the human urine, both in the free state and as its glucuronide. In dog, unusual glucoside conjugates of three metabolites (4''- and 5''-hydroxy and 6-oxo-CBD), not excreted in the unconjugated state, were found as the major metabolites early after drug administration. Other metabolites in all 3 species were mainly acids. Side-chain hydroxylated derivs. of CBD-7-oic acid were particularly abundant in the human urine but much less so in the dog. In the latter species the major oxidized metabolites were the products of beta-oxidation with further hydroxylation at C-6. A related undefined pathway resulted in a loss of 3 carbon atoms from the side-chain of CBD in man, with the production of 2''-hydroxy-tris-nor-CBD-7-oic acid. The 3''-hydroxy metabolites are precursors of compds. having this side-chain. Metabolism by the epoxide-diol pathway, resulting in dihydrodiol formation from the delta-8-double bond, gave metabolites in both dog and human urines. CBD could be used as a probe of the mechanism of several types of biotransformation, particularly those related to carboxylic acid metabolism, as intermediates of a type not usually seen with endogenous compds. were excreted in substantial concentration

IT 63958-72-5 63958-79-2 63958-82-7
 127876-08-0 127876-09-9 131419-44-8
 131419-46-0 131419-47-1 132587-88-3
 132587-91-8 132587-93-0 132587-94-1
 132587-95-2 132587-96-3 132587-97-4
 132587-98-5 132587-99-6 132588-00-2
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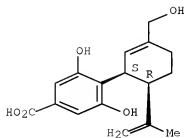
RL: BIOL (Biological study)

(of urine, as cannabidiol metabolite, in humans and laboratory animals)

RN 63958-72-5 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

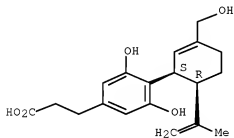
Absolute stereochemistry.



RN 63958-79-2 CAPLUS

CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

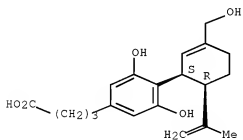
Absolute stereochemistry.



RN 63958-82-7 CAPLUS

CN Benzenobutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

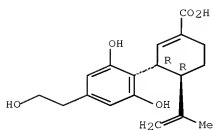
Absolute stereochemistry.



RN 127876-08-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

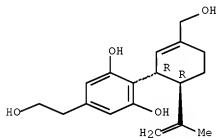
Absolute stereochemistry.



RN 127876-09-9 CAPLUS

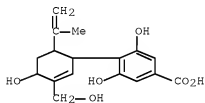
CN 1,3-Benzenediol, 5-(2-hydroxyethyl)-2-(3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl)-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



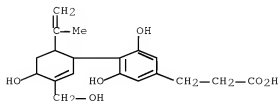
RN 131419-44-8 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-46-0 CAPLUS

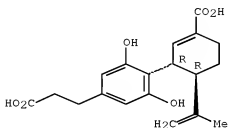
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-47-1 CAPLUS

CN Benzenepropanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

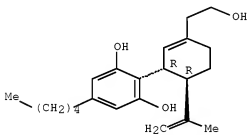
Absolute stereochemistry.



RN 132587-88-3 CAPLUS

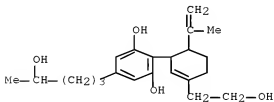
CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



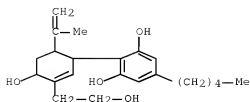
RN 132587-91-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



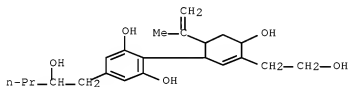
RN 132587-93-0 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



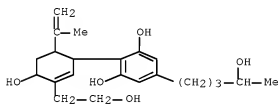
RN 132587-94-1 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)



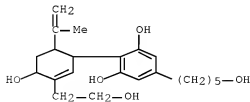
RN 132587-95-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 132587-96-3 CAPLUS

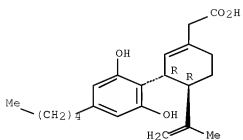
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)



RN 132587-97-4 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

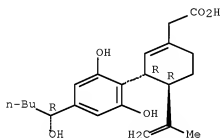
Absolute stereochemistry.



RN 132587-98-5 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

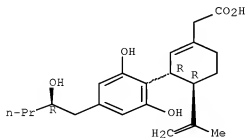
Absolute stereochemistry.



RN 132587-99-6 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

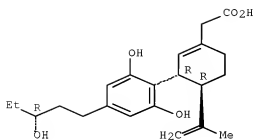
Absolute stereochemistry.



RN 132588-00-2 CAPLUS

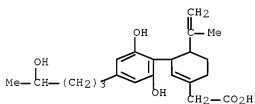
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132588-01-3 CAPLUS

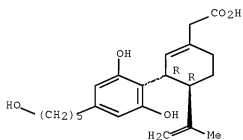
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 132588-02-4 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(5-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (3R-trans)- (9CI) (CA INDEX NAME)

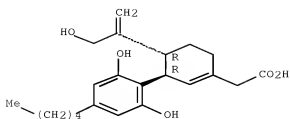
Absolute stereochemistry.



RN 132588-03-5 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-[1-(hydroxymethyl)ethenyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

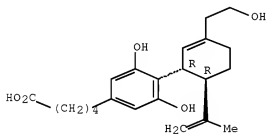
Absolute stereochemistry.



RN 132588-04-6 CAPLUS

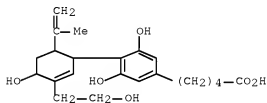
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132588-07-9 CAPLUS

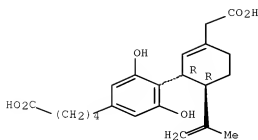
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 132588-08-0 CAPLUS

CN Benzenepentanoic acid, 4-[3-(carboxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

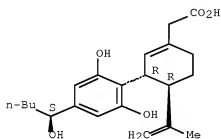
Absolute stereochemistry.



RN 132620-84-9 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

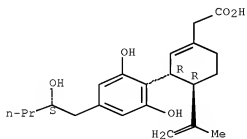
Absolute stereochemistry.



RN 132620-85-0 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

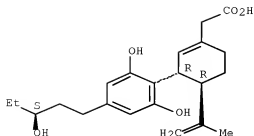
Absolute stereochemistry.



RN 132620-86-1 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L17 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:135490 CAPLUS Full-text

DOCUMENT NUMBER: 114:135490

ORIGINAL REFERENCE NO.: 114:22789a,22792a

TITLE: Urinary metabolites of cannabidiol in dog, rat and man and their identification by gas chromatography-mass spectrometry

AUTHOR(S): Harvey, D. J.; Samara, E.; Mechoulam, R.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK

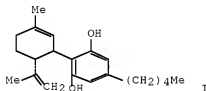
SOURCE: Journal of Chromatography, Biomedical Applications (1991), 562(1-2), 299-322

CODEN: JCBADL; ISSN: 0378-4347

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Urinary metabolites of cannabidiol (I) (CBD), a non-psychoactive cannabinoid of potential therapeutic interest, were extracted from dog, rat, and human urine, concentrated by chromatog. on Sephadex LH-20 and examined by gas chromatog.-mass spectrometry as trimethylsilyl (TMS), [2H9]TMS, Me ester-TMS and methyloxime-TMS derivs. Fragmentation of the metabolites under electron-impact gave structurally informative fragment ions; computer-generated single-ion plots of these diagnostic ions were used extensively to aid metabolite identification. Over 50 metabolites were identified with considerable species variation. CBD was excreted in substantial concentration in human urine, in the free state and as its glucuronide. In dog, unusual glucoside conjugates of 3 metabolites (4''- and 5''-hydroxy- and 6-oxo-CBD), not excreted in the unconjugated state, were found as the major metabolites at early times after drug administration. Other metabolites in all 3 species were mainly acids. Side-chain hydroxylated derivs. of CBD-7-oic acid were particularly abundant in human urine but much less so in dog. In the latter species, the major oxidized metabolites were the products of β -oxidation with further hydroxylation at C-6. A related, but undefined pathway resulted in loss of 3

carbon atoms from the side-chain of CBD in man with production of 2''-hydroxy-tris,nor-CBD-7-oic acid. Metabolism by the epoxide-diol pathway, resulting in dihydro-diol formation from the Δ-8 double bond, gave metabolites in dog and human urine. Thus, CBD could be used as a probe of the mechanism of several types of biotransformation: particularly those related to carboxylic acid metabolism as intermediates of the type not usually seen with endogenous compds. were excreted in substantial concentration

IT 63958-72-5 63958-73-2 63958-62-7
 127876-06-8 127876-09-9 131419-44-8
 131419-46-0 131419-47-1 132587-08-3
 132587-91-8 132587-93-0 132587-94-1
 132587-95-2 132587-96-3 132587-97-4
 132587-98-5 132587-99-6 132588-00-2
 132588-01-3 132588-02-4 132588-03-5
 132588-04-6 132588-07-9 132588-08-0
 132620-04-9 132620-85-0 132620-86-1

RL: ANT (Analyte); ANST (Analytical study)

(determination of, as cannabidiol metabolite, in urine of humans and

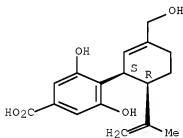
laboratory

animals by gas chromatog.-mass spectrometry)

RN 63958-72-5 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

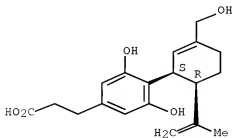
Absolute stereochemistry.



RN 63958-79-2 CAPLUS

CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

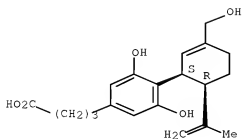
Absolute stereochemistry.



RN 63958-82-7 CAPLUS

CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

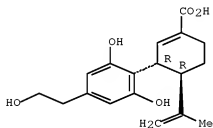
Absolute stereochemistry.



RN 127876-08-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

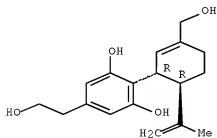
Absolute stereochemistry.



RN 127876-09-9 CAPLUS

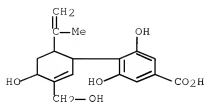
CN 1,3-Benzenediol, 5-(2-hydroxyethyl)-2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



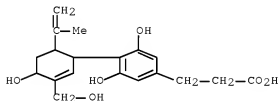
RN 131419-44-8 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-46-0 CAPLUS

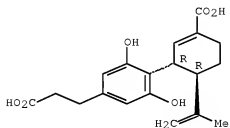
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-47-1 CAPLUS

CN Benzenepropanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

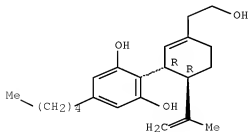
Absolute stereochemistry.



RN 132587-88-3 CAPLUS

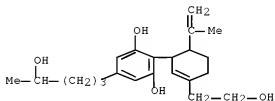
CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



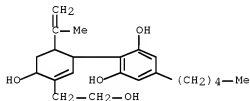
RN 132587-91-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



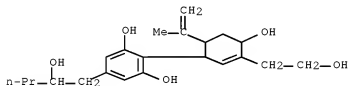
RN 132587-93-0 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



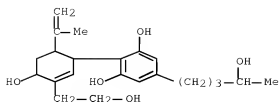
RN 132587-94-1 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)



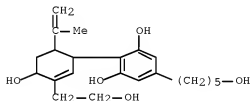
RN 132587-95-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 132587-96-3 CAPLUS

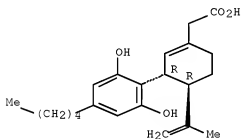
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)



RN 132587-97-4 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

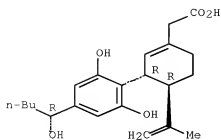
Absolute stereochemistry.



RN 132587-98-5 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

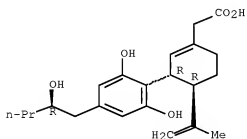
Absolute stereochemistry.



RN 132587-99-6 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

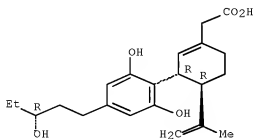
Absolute stereochemistry.



RN 132588-00-2 CAPLUS

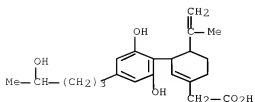
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132588-01-3 CAPLUS

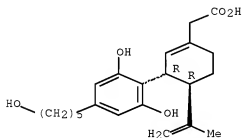
CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 132588-02-4 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(5-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

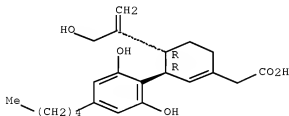
Absolute stereochemistry.



RN 132588-03-5 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-[1-(hydroxymethyl)ethenyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

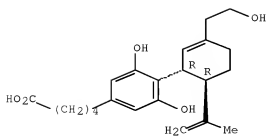
Absolute stereochemistry.



RN 132588-04-6 CAPLUS

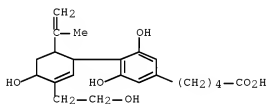
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132588-07-9 CAPLUS

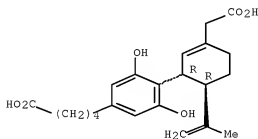
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(2-hydroxyethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 132588-08-0 CAPLUS

CN Benzenepentanoic acid, 4-[3-(carboxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

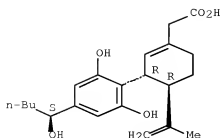
Absolute stereochemistry.



RN 132620-84-9 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

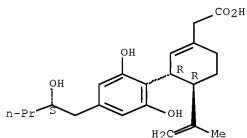
Absolute stereochemistry.



RN 132620-85-0 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

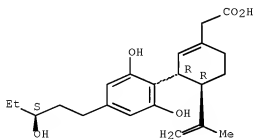
Absolute stereochemistry.



RN 132620-86-1 CAPLUS

CN 1-Cyclohexene-1-acetic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*),4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L17 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:94580 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 114:94580

ORIGINAL REFERENCE NO.: 114:15915a,15918a

TITLE: Pharmacokinetics of urinary metabolites of cannabidiol in the dog

AUTHOR(S): Samara, Emil; Bialer, Meir; Harvey, David J.

CORPORATE SOURCE: Sch. Pharm., Hebrew Univ., Jerusalem, 91120, Israel
SOURCE: Biopharmaceutics & Drug Disposition (1990), 11(9),
785-95
CODEN: BDDID8; ISSN: 0142-2782

DOCUMENT TYPE: Journal
LANGUAGE: English

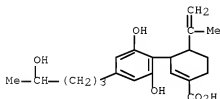
AB The pharmacokinetics of cannabidiol (CBD) and 6 of its urinary metabolites were investigated in dogs. CBD was administered i.v. to dogs, and urine was collected at specified time intervals over a period of 30 h. The apparent terminal half-life of CBD calculated from the slope of the sigma minus plot was shorter (2 h) than the half-life of CBD calculated from plasma data (8 h), and the apparent terminal half-life of the metabolites was similar to that of the CBD calculated from plasma data, indicating that the elimination of these metabolites was formation rate limited. The time course of the metabolite excretion could be divided into 2 phases: the first phase contained mainly monohydroxy metabolites, and the second phase contained mainly metabolites with a carboxylic acid moiety in their side-chain.

IT 63958-84-9 130413-92-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(pharmacokinetics of, as cannabidiol urinary metabolite)

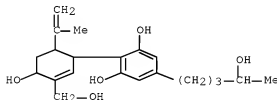
RN 63958-84-9 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 130413-92-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L17 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:55236 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 114:55236

ORIGINAL REFERENCE NO.: 114:9297a,9300a

TITLE: Identification of urinary metabolites of cannabidiol

in the dog
 AUTHOR(S): Samara, E.; Bialer, M.; Harvey, D. J.
 CORPORATE SOURCE: Dep. Pharmacol., Oxford Univ., Oxford, OX1 3QT, UK
 SOURCE: Drug Metabolism and Disposition (1990), 18(5), 571-9
 CODEN: DMSDAI; ISSN: 0090-9556
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Dogs were treated with cannabidiol (CBD) and urine samples were collected for 30 h. Metabolites were extracted with Et acetate before and after hydrolysis with β -glucuronidase, and examined by GC-MS. Thirty-seven metabolites were identified and 9 partially characterized; 21 of the identified metabolites have not been reported before. The major oxidative metabolic routes were 6-hydroxylation, both α and β , and β -oxidation. At 10 h, the major metabolites of this type were 6-hydroxy-4'',5''-bis-nor-CBD-3''-oic acid and 6-oxo-4'',5''-bis-nor-CBD-3''-oic acid, whereas at 22 h, further β -oxidation had occurred to give 6-hydroxy-2'',3'',4'',5''-tetrakis,nor-CBD-1''-oic acid as the major metabolite. Other metabolic routes were carboxylic acid formation at C-7 accompanied by hydroxylation in the side chain, and dihydroxylation of the C-8,9 double bond. Three compds., 4''-hydroxy-CBD, 5''-hydroxy-CBD, and 6-oxo-CBD were found at early times as glucose conjugates in concns. that exceeded those of the other metabolites. The unconjugated forms of these metabolites were not found and none of the identified oxidized metabolites were found glucosides. Only 4'',5-dihydroxy-CBD was found conjugated with glucuronic acid.

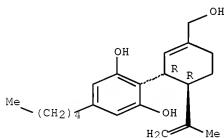
IT 50725-17-2 61361-39-5 61361-42-0
 63958-79-2 63958-80-5 63958-84-9
 63958-85-0 130413-92-2 130413-93-3
 131419-41-5 131419-44-8 131419-46-0
 131419-47-1 131419-49-3 131419-50-6

RL: BIOL (Biological study)
 (of urine, as cannabidiol metabolite)

RN 50725-17-2 CAPLUS

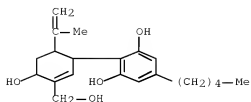
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



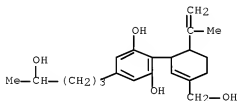
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

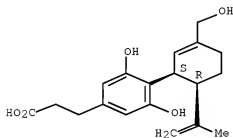
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 63958-79-2 CAPLUS

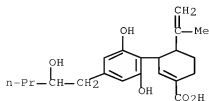
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



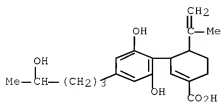
RN 63958-80-5 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-84-9 CAPLUS

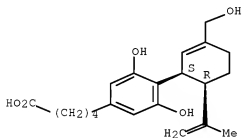
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-85-0 CAPLUS

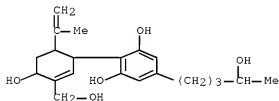
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



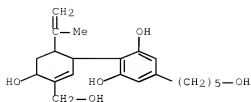
RN 130413-92-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



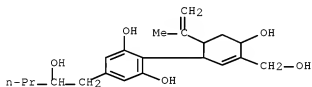
RN 130413-93-3 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)



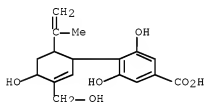
RN 131419-41-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)



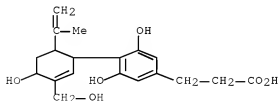
RN 131419-44-8 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-46-0 CAPLUS

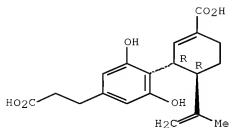
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-47-1 CAPLUS

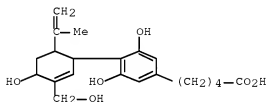
CN Benzenepropanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 131419-49-3 CAPLUS

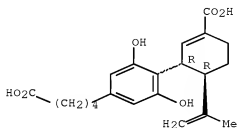
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)



RN 131419-50-6 CAPLUS

CN Benzenepentanoic acid, 4-[3-carboxy-6-(1-methylethenyl)-2-cyclohexen-1-yl]-3,5-dihydroxy-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:624061 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:224061

ORIGINAL REFERENCE NO.: 113:37617a,37620a

TITLE: In vitro metabolism of cannabidiol in the rabbit: identification of seventeen new metabolites including thirteen dihydroxylated in the isopropenyl chain Harvey, D. J.; Brown, N. K.

AUTHOR(S): Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK

SOURCE: Biomedical & Environmental Mass Spectrometry (1990),

19(9), 559-67

CODEN: BEMSEN; ISSN: 0887-6134

DOCUMENT TYPE:

Journal

LANGUAGE:

English

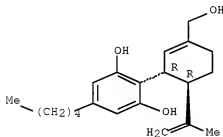
AB The metab. of cannabidiol (CBD) was studied in liver microsomes from the female New Zealand white rabbit. Metabolites were extracted with Et acetate, concentrated by chromatog. on Sephadex LH 20, and examined as trimethylsilyl (TMS), Me ester/TMS, and (2H9)TMS derivs. by GC/mass spectrometry. Thirty-nine metabolites, mainly mono-, di- and tri-hydroxy compds., were identified; 17 of these have not been reported before. New metabolites included 8,9-dihydro-CBD (two isomers) and seven monohydroxy derivs. of each of these two compds. The mass spectra of the TMS derivs. of metabolites not hydroxylated in the isopropenyl group were generally dominated by the ion produced by retro-Diels-Alder cleavage of the terpene ring. Other structurally informative ions included the tropylium ion and fragments diagnostic of hydroxylation at C-1", C-2", C-3", C-4" and C-7. The spectra of the TMS derivs. of metabolites hydroxylated in the isopropenyl group were generally dominated by the ion at m/z 143. This involved loss of CH₂OTMS and a retro-Diels-Alder fragmentation analogous to that seen in the other metabolites, but with charge retention by the other (smaller) fragment. Other, related fragment ions also characterized these metabolites.

IT 50725-17-2 61361-39-5 61361-41-9
61361-42-0 61361-43-1 130413-99-0
130413-91-1 130413-92-2 130413-93-3
130467-21-9 130467-22-0
RL: BIOL (Biological study)
(as cannabidiol metabolite, in liver)

RN 50725-17-2 CAPLUS

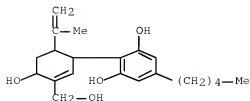
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



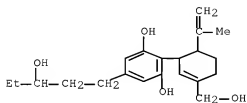
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



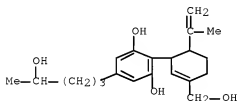
RN 61361-41-9 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

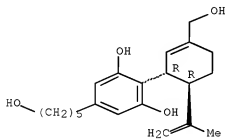
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 61361-43-1 CAPLUS

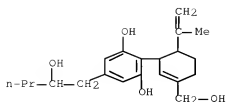
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



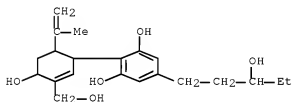
RN 130413-90-0 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(2-hydroxypentyl)- (CA INDEX NAME)



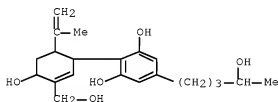
RN 130413-91-1 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)



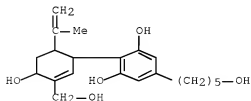
RN 130413-92-2 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 130413-93-3 CAPLUS

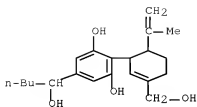
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)- (CA INDEX NAME)



RN 130467-21-9 CAPLUS

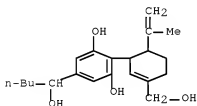
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)-, [1R-[1α(R*),2β]]- (9CI) (CA INDEX NAME)

NAME)



RN 130467-22-0 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)-, [2R-[2α(S*),3β]]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:624057 CAPLUS Full-text

DOCUMENT NUMBER: 113:224057

ORIGINAL REFERENCE NO.: 113:37616h,37617a

TITLE: In vitro metabolism of cannabidiol in seven common laboratory mammals

AUTHOR(S): Harvey, D. J.; Brown, N. K.

CORPORATE SOURCE: Univ. Dep. Pharmacol., Oxford, OX1 3QT, UK

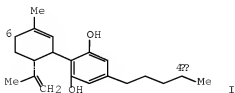
SOURCE: Research Communications in Substances of Abuse (1990), 11(1-2), 27-37

CODEN: RCSADO; ISSN: 0193-0818

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The metab. of cannabidiol (CBD, I) was studied in rat, mouse, rabbit, guinea pig, cat, gerbil, and hamster. Metabolites were extracted from hepatic microsomal preps. with Et acetate, concentrated by chromatog. on Sephadex LH-20 and examined as trimethylsilyl (TMS) and [2H9]TMS derivs. by GC/MS. The identified metabolites were mainly mono- and di-hydroxy compds. and their relative concns. were found to differ considerably between the seven species. 10-Hydroxy-CBD was newly characterized by mass spectrometry; this compound was the major metabolite in the hamster. 7-Hydroxy-CBD was the major metabolite in the mouse, rat, and rabbit whereas the gerbil and guinea-pig favored hydroxylation at C-4''. The cat, on the other hand, gave 6-hydroxy-CBD as the major metabolite. Low concns. of new metabolites, dihydroxylated in the isopropenyl group were also identified in hamster and in the female rabbit: these appeared to have arisen from an intermediate epoxide.

IT 50725-17-2 61361-39-5 61361-42-0

130548-70-8

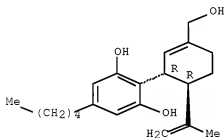
RL: PRP (Properties)

(characterization of, as cannabidiol hydroxylation metabolite, species differences in)

RN 50725-17-2 CAPLUS

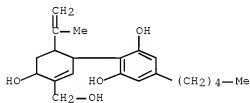
CN 1,3-Benzenediol, 2-[1,3-(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



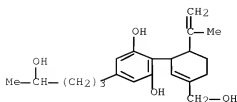
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

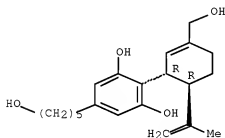
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 130548-70-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L17 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:544804 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:144804

ORIGINAL REFERENCE NO.: 113:24373a,24376a

TITLE: Microsomal metabolism of the 1'',1''-dimethylheptyl analog of cannabidiol: relative percentage of monohydroxy metabolites in four species

AUTHOR(S): Samara, E.; Brown, N. K.; Harvey, D. J.

CORPORATE SOURCE: Dep. Pharm., Hebrew Univ., Jerusalem, Israel

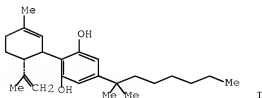
SOURCE: Drug Metabolism and Disposition (1990), 18(4), 548-9

CODEN: DMDSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB The metab. of 1'',1''-dimethylheptylcannabidiol (I) in vitro in liver microsomes from mice, rats, guinea pigs, and rabbits was compared. Species differences were noted in the formation of monohydroxy metabolites of I.

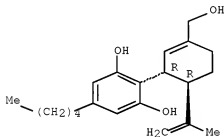
IT 50725-17-2, 7-Hydroxycannabidiol 128395-01-7

RL: FORM (Formation, nonpreparative)
(formation of, as cannabidiol analog metabolite by liver microsome, species differences in)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

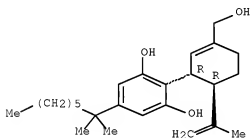
Absolute stereochemistry. Rotation (-).



RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:508661 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:108661

ORIGINAL REFERENCE NO.: 113:18173a,18176a

TITLE: Oxidative cleavage of the pentyl side-chain of cannabinoids: identification of new biotransformation pathways in the metabolism of 4'-hydroxy-delta-9-tetrahydrocannabinol in the mouse Harvey, D. J.

AUTHOR(S): Harvey, D. J.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK

SOURCE: Drug Metabolism and Disposition (1990), 18(3), 350-5

CODEN: DMSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

AB During an investigation of the mechanisms leading to the formation of metabolites of cannabinoids in which the pentyl side chain is reduced to 2, 3 or 4 carbon atoms, the further metabolism of 4'-hydroxy- Δ^9 -tetrahydrocannabinol was investigated in vivo in mice. Metabolites were extracted with Et acetate, concentrated by chromatog. on Sephadex LH-20 and identified by GC/MS. Ten metabolites were identified and a further two had tentative structural assignments made. The major metabolic route, in common with that seen with most cannabinoids, was hydroxylation at the allylic 11-position, followed by oxidation to a carboxylic acid. Addnl. hydroxylation occurred at C-8. Abundant metabolites were also formed by oxidative cleavage of the pentyl side chain. The major metabolites of this type had lost the terminal two carbon atoms to give compds. containing a carboxyethyl side chain. This is the major product normally produced by β -oxidation of the acid formed from 5'-hydroxy- Δ^9 -tetrahydrocannabinol. Trace concns. of 2 other acids that appeared to have a carboxypropyl side chain were also found. The results show that, in addition to β -oxidation, initiated by hydroxylation at the 5'-carbon atom (ω -hydroxylation), at least one other oxidative route, initiated by ω -1-hydroxylation, is involved in the production of metabolites with 2 carbon atoms missing from the pentyl side chain. This pathway does not seem to have been characterized as a biotransformation mechanism in drug metabolism and a possible mechanism is suggested.

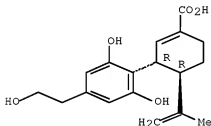
IT 127876-06-8

RL: BIOL (Biological study)
(as hydroxytetrahydrocannabinol metabolite)

RN 127876-08-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L17 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:452013 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:52013

ORIGINAL REFERENCE NO.: 113:8625a,8628a

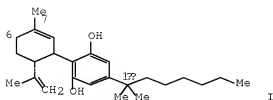
TITLE: Identification of metabolites of the 1',1''-dimethylheptyl analog of cannabidiol in rat and dog in vivo

AUTHOR(S): Samara, E.; Bialer, M.; Bar-On, H.; Harvey, D. J.

CORPORATE SOURCE: Dep. Pharm., Hebrew Univ. Jerusalem, Jerusalem, 91120, Israel

SOURCE: Xenobiotica (1990), 20(5), 447-55
CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Metab. of the 1'',1''-dimethylheptyl analog of cannabidiol (DMH-CBD) (I) was studied using an isolated perfused rat liver preparation and in rat and dog urine. Metabolites were converted into trimethylsilyl (TMS), Me ester/TMS and [2H9]TMS derivs. and gas chromatog.-mass spectrometry. In contrast with the metabolism of cannabidiol, the dimethylheptyl analog gas low concns. of metabolites in all media examined. Four metabolites were found in the perfusion fluid. Two were identified as 6- and 7-hydroxy-DMH-CBD and the other two were found to be hydroxylated in the dimethylheptyl chain but at undetd. positions. Five metabolites were identified in dog urine; these were the 6- and 7-mono-hydroxy and 6,7-dihydroxy derivs. of acids formed by one stage of β -oxidation of the dimethylheptyl chain, and the 6- and 7-hydroxy derivs. of corresponding acids formed by loss of three carbon atoms from the chain. Metabolic routes were very similar to those found earlier for cannabidiol.

IT 128366-72-3 128366-74-5 128366-75-6
 128395-01-7

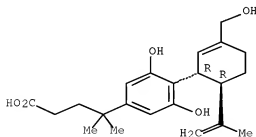
RL: FORM (Formation, nonpreparative)

(formation of, as metabolite of cannabidiol dimethylheptyl analog, in liver and urine)

RN 128366-72-3 CAPLUS

CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- γ,γ -dimethyl-, (1R-trans)-(9CI) (CA INDEX NAME)

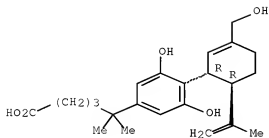
Absolute stereochemistry.



RN 128366-74-5 CAPLUS

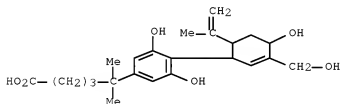
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- δ,δ -dimethyl-, (1R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 128366-75-6 CAPLUS

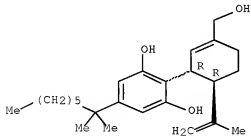
CN Benzenepentanoic acid, 3,5-dihydroxy-4-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-8,8-dimethyl- (CA INDEX NAME)



RN 128395-01-7 CAPLUS

CN 1,3-Benzenediol, 5-(1,1-dimethylheptyl)-2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L17 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1990:434276 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:34276

ORIGINAL REFERENCE NO.: 113:5685a,5688a

TITLE: Metabolites of cannabidiol identified in human urine

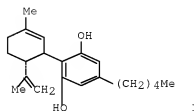
AUTHOR(S): Harvey, D. J.; Mechoulam, R.

CORPORATE SOURCE:
SOURCE:

Univ. Dep. Pharmacol., Oxford, OX1 3QT, UK
Xenobiotica (1990), 20(3), 303-20
CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



I

AB Urine from a dystonic patient treated with cannabidiol (I) was examd. by gas chromatog.-mass spectrometry for I metabolites. Metabolites were identified as their trimethylsilyl (TMS), [2H₉]TMS, and Me ester/TMS derivs. and as the TMS derivs. of the product of lithium aluminum deuteride reduction. Thirty-three metabolites were identified in addition to unmetabolized I, and a further four metabolites were partially characterized. The major metabolic route was hydroxylation and oxidation at C-7 followed by further hydroxylation in the pentyl and propenyl groups to give 1"-, 2"-, 3"-, 4"- and 10-hydroxy derivs. of I-7-oic acid. Other metabolites, mainly acids, were formed by β -oxidation and related biotransformations from the pentyl side-chain and these were also hydroxylated at C-6 or C-7. The major oxidized metabolite was I-oic acid containing a hydroxyethyl side-chain. Two 8,9-dihydroxy compds., presumably derived from the corresponding epoxide were identified. Also present were several cyclized cannabinoids including Δ -6- and Δ -1-tetrahydrocannabinol and cannabinol. This is the first metabolic study of I in humans, most observed metabolic routes were typical of those found for I and related cannabinoids in other species.

IT 50725-17-2 61361-39-5 63958-72-5
63958-77-0 63958-79-2 63958-82-7
63958-84-9 63958-85-0 127876-00-0
127876-01-1 127876-08-8 127876-09-9
127913-37-5 127913-38-6 127913-39-7
127913-40-0 127913-41-1

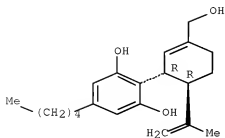
RL: PROC (Process)

(identification of, as cannabidiol metabolite, in human urine, by gas chromatog.-mass spectrometry)

RN 50725-17-2 CAPLUS

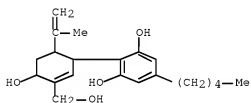
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 61361-39-5 CAPLUS

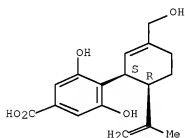
CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



RN 63958-72-5 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

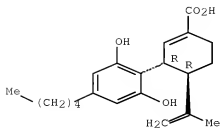
Absolute stereochemistry.



RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

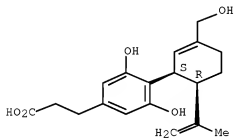
Absolute stereochemistry. Rotation (-).



RN 63958-79-2 CAPLUS

CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

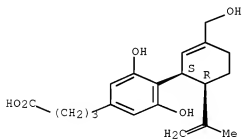
Absolute stereochemistry.



RN 63958-82-7 CAPLUS

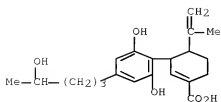
CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 63958-84-9 CAPLUS

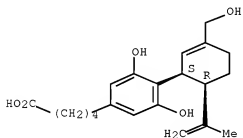
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-85-0 CAPLUS

CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

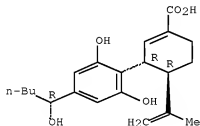
Absolute stereochemistry.



RN 127876-00-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*),4β]]-(9CI) (CA INDEX NAME)

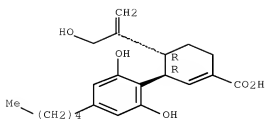
Absolute stereochemistry.



RN 127876-01-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-[1-(hydroxymethyl)ethenyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

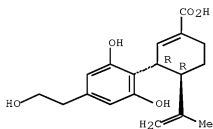
Absolute stereochemistry.



RN 127876-08-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxyethyl)phenyl]-4-(1-methylethenyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

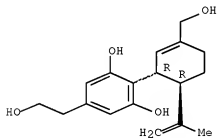
Absolute stereochemistry.



RN 127876-09-9 CAPLUS

CN 1,3-Benzenediol, 5-(2-hydroxyethyl)-2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1R-trans)- (9CI) (CA INDEX NAME)

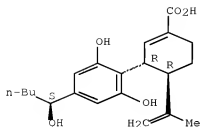
Absolute stereochemistry.



RN 127913-37-5 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(1-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*), 4β]]-(9CI) (CA INDEX NAME)

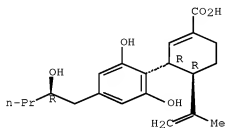
Absolute stereochemistry.



RN 127913-38-6 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*), 4β]]-(9CI) (CA INDEX NAME)

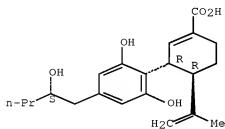
Absolute stereochemistry.



RN 127913-39-7 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*), 4β]]-(9CI) (CA INDEX NAME)

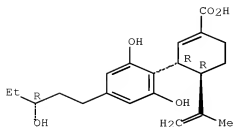
Absolute stereochemistry.



RN 127913-40-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(R*), 4β]]-(9CI) (CA INDEX NAME)

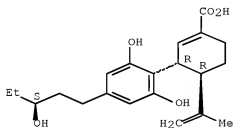
Absolute stereochemistry.



RN 127913-41-1 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)-, [3R-[3α(S*), 4β]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L17 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:127977 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 110:127977

ORIGINAL REFERENCE NO.: 110:20919a, 20922a

TITLE: Identification of cannabidiol, a new metabolite of cannabidiol formed by guinea pig hepatic microsomal enzymes, and its pharmacological activity in mice
Yamamoto, Ikuo; Gohda, Hiroshi; Narimatsu, Shizuo; Yoshimura, Hidetoshi

AUTHOR(S): Sch. Pharm., Hokuriku Univ., Kanagawa, 920-11, Japan
CORPORATE SOURCE: Journal of Pharmacobio-Dynamics (1988), 11(12), 833-8
SOURCE: CODEN: JOPHDQ; ISSN: 0386-846X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The metab. of cannabidiol (CBD), one of the major components of marijuana, was studied in the guinea pig both in vitro and in vivo. Analyses of metabolites by gas chromatog. and gas chromatog.-mass spectrometry proved that cannabidiol (CBE) was formed from CBD as a novel metabolite, and that the amount was about one-sixth that of 7-hydroxy-CBD, which was the most abundant metabolite under in vitro conditions in the presence of microsomal monooxygenase (cytochrome P 450). CBE was also found in the liver of guinea pigs given CBD (100 mg/kg) i.p. 1 h before sacrifice. In mice, CBE had little activity on pentobarbital-induced sleep and body temperature

IT 50725-17-2, 7-Hydroxycannabidiol

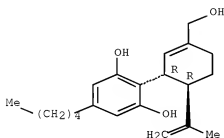
RL: FORM (Formation, nonpreparative)

(formation of, as cannabidiol metabolite, by liver microsome)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L17 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1985:433115 CAPLUS Full-text

DOCUMENT NUMBER: 103:33115

ORIGINAL REFERENCE NO.: 103:5299a,5302a

TITLE: Studies on confirmation of cannabis use. I.
Determination of the cannabinoid contents in marijuana
cigarette, tar, and ash using high performance liquid
chromatography with electrochemical detection

AUTHOR(S): Nakahara, Yuji; Sekine, Hitoshi
CORPORATE SOURCE: Natl. Res. Inst. Police Sci., Tokyo, 102, Japan
SOURCE: Journal of Analytical Toxicology (1985), 9(3), 121-4
CODEN: JATOD3; ISSN: 0146-4760

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A HPLC-electrochem. detection (HPLC-ECD) method was used for the highly sensitive and simultaneous determination of free cannabinoids and cannabinoic acids without derivatization. The HPLC-ECD method was linear from 5 to 500 ng/injection for all cannabinoids [Δ^9 -tetrahydrocannabinol (I) [1972-08-3], cannabinol [521-35-7], cannabidiol [13956-29-1], cannabichromene [20675-51-8], Δ^9 -tetrahydrocannabinolic acid (II) [56354-06-4], cannabidiolic acid [63958-77-0], and cannabichromenic acid [20408-52-0]]. The detection limits of this method were 0.5-0.9 ng/injection for free cannabinoids and 1.2-2.5 ng/injection for cannabinoic acids at a signal noise ratio of >4. Cannabinoic contents in marijuana cigarettes and in tar and ash obtained by using an automatic smoking machine were measured by this method. Consequently, 62% of the sum of I and II in the marijuana cigarette was converted to tar and 2.0% of that was left in the ash.

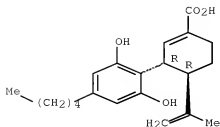
IT 63958-77-0

RL: ANT (Analyte); ANST (Analytical study)
(determination of, in marijuana ash and smoke and tar, by HPLC with
electrochem. detection)

RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L17 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1980:488375 CAPLUS Full-text

DOCUMENT NUMBER: 93:88375

ORIGINAL REFERENCE NO.: 93:13999a,14002a

TITLE: Identification of in vivo liver metabolites of

Δ^1 -tetrahydrocannabinol, cannabidiol, and
cannabinol produced by the guinea pig

AUTHOR(S): Harvey, D. J.; Martin, B. R.; Paton, W. D. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, OX1 3QT, UK

SOURCE: Journal of Pharmacy and Pharmacology (1980), 32(4),
267-71

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By combined gas chromatog.-mass spectrometry, 45 metabolites of Δ^1 -tetrahydrocannabinol (I) [1972-08-3] were identified in liver from guinea pigs given a 100 mg/kg i.p. dose. The major metabolic routes involved allylic and aliphatic hydroxylations, oxidns. to ketones and acids, oxidative degradation of the side chain presumably by the β -oxidation path, and formation of glucuronide conjugates. Di- and tri-substituted metabolites were abundant. The 1-hydroxy-derivative of I was observed as a pair of diastereoisomers. Similar metabolic paths were observed with cannabidiol [13956-29-1]; 20 metabolites were identified. Only 6 metabolites of cannabinol [521-35-7] were identified; these were mainly mono-substituted derivs.

IT 50725-17-2 61361-40-8 61361-41-9

61361-42-0 63958-77-0 63958-79-2

63958-84-9 63958-85-0 74513-76-1

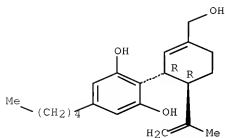
RL: BIOL (Biological study)

(as cannabidiol metabolite)

RN 50725-17-2 CAPLUS

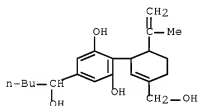
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



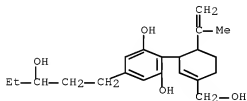
RN 61361-40-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)- (CA INDEX NAME)



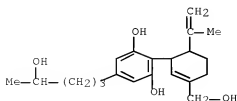
RN 61361-41-9 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

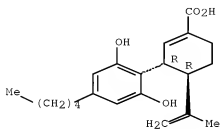
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

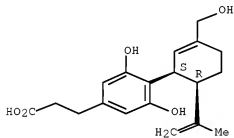
Absolute stereochemistry. Rotation (-).



RN 63958-79-2 CAPLUS

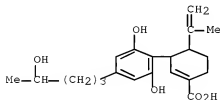
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 63958-84-9 CAPLUS

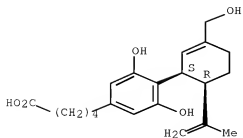
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-85-0 CAPLUS

CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

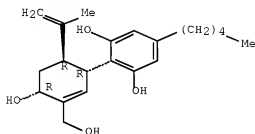
Absolute stereochemistry.



RN 74513-76-1 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, [1R-(1a,4a,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L17 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1978:608839 CAPLUS Full-text

DOCUMENT NUMBER: 89:208839

ORIGINAL REFERENCE NO.: 89:32303a,32306a

TITLE: Comparative in vivo metabolism of Δ1-tetrahydrocannabinol (Δ1-THC), cannabidiol (CBD) and cannabinol (CBN) by several species

AUTHOR(S): Harvey, D. J.; Martin, B. R.; Paton, W. D. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, UK

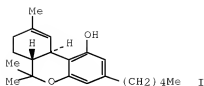
SOURCE: Recent Dev. Mass Spectrom. Biochem. Med., [Proc. Int. Symp.], 4th (1978), Meeting Date 1977, Volume 1, 161-84. Editor(s): Frigerio, Alberto. Plenum: New York, N. Y.

CODEN: 38XPAL

DOCUMENT TYPE: Conference

LANGUAGE: English

GI



AB The metab. of Δ^1 -tetrahydrocannabinol (I) [1972-08-3], cannabidiol (II) [13956-29-1], and cannabinol (III) [521-35-7] was studied in mice, rats, and guinea pigs. I was extensively metabolized to mono-, di-, and triols, hydroxy and dihydroxy ketones, acids, hydroxy and dihydroxy acids, and dihydro compds. Three new metabolites of I were identified: α - [64663-37-2] and β -hexahydrocannabinolic acid [64663-38-3] and the O-glucuronide [62726-09-4]. Guinea pigs produced large amts. of side-chain acids and compds. containing 6 β substitution, whereas mice produced mainly 7-substituted metabolites. Glucuronide formation was the major metabolic route for II and III. II and III also produced monohydroxy and dihydroxy metabolites, carboxylic acids and hydroxy carboxylic acids. In contrast to I, side-chain acid formation was a major biotransformation route for II in mice and benzylic rather than allylic hydroxylation was most common in III metabolism

IT 59725-17-2 61361-39-5 61361-40-8
 61361-42-0 63958-80-5 63958-83-8
 63958-84-9 68295-92-1 68295-94-3
 68295-96-5 68295-98-7 68295-99-8

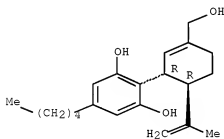
RL: BIOL (Biological study)

(as cannabidiol metabolite, species in relation to)

RN 50725-17-2 CAPLUS

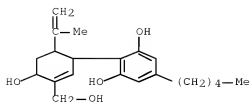
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



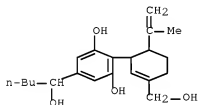
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



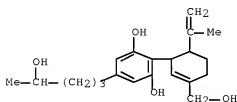
RN 61361-40-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)- (CA INDEX NAME)



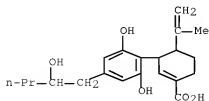
RN 61361-42-0 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



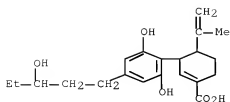
RN 63958-80-5 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



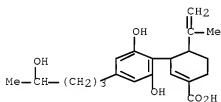
RN 63958-83-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-84-9 CAPLUS

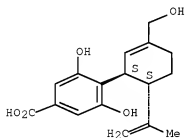
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 68295-92-1 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)

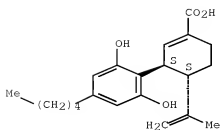
Absolute stereochemistry.



RN 68295-94-3 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3S,4S)- (CA INDEX NAME)

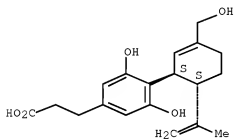
Absolute stereochemistry.



RN 68295-96-5 CAPLUS

CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)

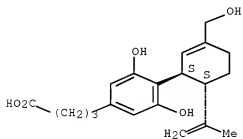
Absolute stereochemistry.



RN 68295-98-7 CAPLUS

CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)

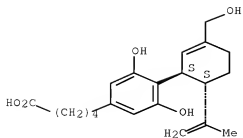
Absolute stereochemistry.



RN 68295-99-8 CAPLUS

CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L17 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:545454 CAPLUS Full-text

DOCUMENT NUMBER: 87:145454

ORIGINAL REFERENCE NO.: 87:22905a,22908a

TITLE: Marihuana metabolites in urine of man. VII.
Excretion patterns of acidic metabolites detected by
sequential thin layer chromatography

AUTHOR(S): Kanter, Saul L.; Hollister, Leo E.

CORPORATE SOURCE: VA Hosp., Palo Alto, CA, USA

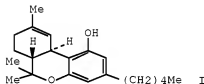
SOURCE: Research Communications in Chemical Pathology and
Pharmacology (1977), 17(3), 421-31

CODEN: RCOCB8; ISSN: 0034-5164

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Using sequential thin-layer chromatog., the 11-oic acid metabolites of Δ^9 -tetrahydrocannabinol (I) [1972-08-3], cannabinol [521-35-7], and cannabidiol [13956-29-1] were identified, presumptively, in the urine of persons taking these materials.

IT 63958-77-0

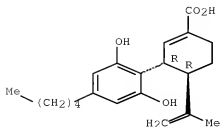
RL: PROC (Process)

(as cannabidiol metabolite, detection of, in urine by thin-layer chromatog.)

RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L17 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:526890 CAPLUS Full-text

DOCUMENT NUMBER: 87:126890

ORIGINAL REFERENCE NO.: 87:20049a,20052a

TITLE: Biotransformation of cannabidiol in mice.

Identification of new acid metabolites

AUTHOR(S): Martin, B. R.; Harvey, D. J.; Paton, W. D. M.

CORPORATE SOURCE: Univ. Dep. Pharmacol., Oxford, UK

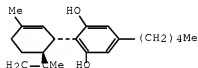
SOURCE: Drug Metabolism and Disposition (1977), 5(3), 259-67

CODEN: DMSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB The in vivo metab. of cannabidiol (I) [13956-29-1] was investigated in mice. Following i.p. administration of I to mice, livers were removed and metabolites were extracted with ethyl acetate prior to partial purification on Sephadex LH-20 columns. Fractions from the columns were converted to trimethylsilyl, d9-trimethylsilyl, and methylester-trimethylsilyl derivs. for anal. by gas-liquid chromatog.-mass spectrometry. In addition metabolites containing carboxylic acid and ketone groups were reduced to alcs. with LiAlD4 before trimethylsilation. A total of 22 metabolites were characterized, 14 of which had not been reported previously. The metabolites can be categorized as: mono- and di-hydroxylated derivs., cannabidiol-7-oic acid [63958-72-5], side chain hydroxylated cannabidiol-7-oic acids, side-chain acids, 7-hydroxy-side-chain acids, 6-oxo-side-chain acids, and glucuronide conjugates. The most significant biotransformations were glucuronide conjugation and, to a lesser extent, formation of cannabidiol-7-oic acid.

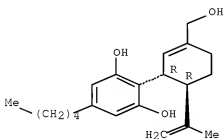
IT 50725-17-2 61361-39-5 61361-40-8
61361-42-0 63958-72-5 63958-77-0
63958-79-2 63958-80-5 63958-82-7
63958-83-8 63958-84-9 63958-85-0

RL: BIOL (Biological study)
(as cannabidiol metabolite)

RN 50725-17-2 CAPLUS

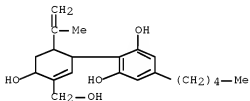
CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



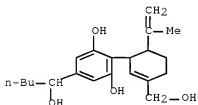
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



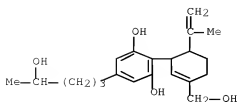
RN 61361-40-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

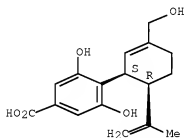
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 63958-72-5 CAPLUS

CN Benzoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

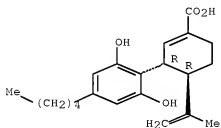
Absolute stereochemistry.



RN 63958-77-0 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-(2,6-dihydroxy-4-pentylphenyl)-4-(1-methylethenyl)-, (3R,4R)- (CA INDEX NAME)

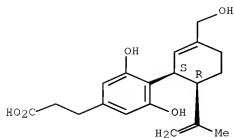
Absolute stereochemistry. Rotation (-).



RN 63958-79-2 CAPLUS

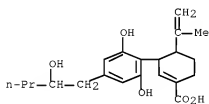
CN Benzenepropanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 63958-80-5 CAPLUS

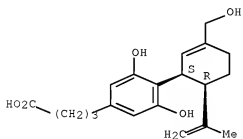
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(2-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-82-7 CAPLUS

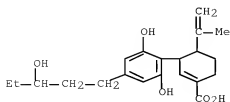
CN Benzenebutanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



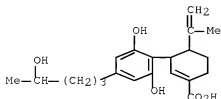
RN 63958-83-8 CAPLUS

CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(3-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-84-9 CAPLUS

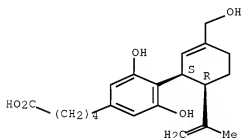
CN 1-Cyclohexene-1-carboxylic acid, 3-[2,6-dihydroxy-4-(4-hydroxypentyl)phenyl]-4-(1-methylethenyl)- (CA INDEX NAME)



RN 63958-85-0 CAPLUS

CN Benzenepentanoic acid, 3,5-dihydroxy-4-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L17 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:400076 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 87:76

ORIGINAL REFERENCE NO.: 87:7a,10a

TITLE: Identification of glucuronides as in vivo liver conjugates of seven cannabinoids and some of their hydroxy and acid metabolites

AUTHOR(S): Harvey, D. J.; Martin, B. R.; Paton, W. D. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, UK

SOURCE: Research Communications in Chemical Pathology and

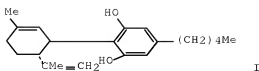
Pharmacology (1977), 16(2), 265-79

CODEN: RCOCB8; ISSN: 0034-5164

DOCUMENT TYPE: Journal

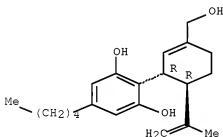
LANGUAGE: English

GI



AB	Glucuronide conjugates of cannabidiol (I), 7-hydroxy-I, propyl-I, cannabinol (CBN) [62667-56-5], 7-hydroxy-CBN, CBN-7-oic acid [62667-57-6], propyl-CBN [62667-58-7] and cannabichromene [62667-59-8] were identified as major metabolites of I, CBN, and their propyl homologs and of cannabichromene in mouse liver. Trace amts. of Δ^1 -[62726-09-4] and $\Delta^1(6)$ -tetrahydrocannabinol glucuronide [62667-60-1] were also detected. Identification was made by combined gas-liquid chromatog. and mass spectrometric studies of the trimethylsilyl (TMS), d9-TMS and Me ester-TMS derivs. of the glucuronides and the TMS derivs. of the product of the reduction of the metabolites with LiAlD4.
IT	50725-17-2D, glucuronide RL: BIOL (Biological study) (as cannabinoid metabolite)
RN	50725-17-2 CAPLUS
CN	1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L17 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:25791 CAPLUS Full-text

DOCUMENT NUMBER: 86:25791

ORIGINAL REFERENCE NO.: 86:4047a, 4050a

TITLE: Identification of the glucuronides of cannabidiol and hydroxycannabidiols in mouse liver

AUTHOR(S) : Harvey, D. J.; Martin, B. R.; Paton, W. D. M.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Oxford, Oxford, UK

SOURCE: Biochemical Pharmacology (1976), 25(19), 2217-19

CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

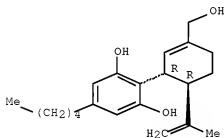
LANGUAGE: English

AB After treatment of mice with cannabidiol (I) [13956-29-1] (100 mg/kg, i.p.) a gas-liquid chromatog. profile of the metabolites extracted from the livers and converted to trimethylsilyl derivs. contained a group of peaks identified as conjugates with retention times from 38-50 min. Mass spectroscopic studies of

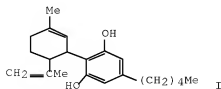
the most abundant conjugate suggested that it probably contained glucuronic acid. Hydrolysis of the metabolic fraction with β -glucuronidase at pH 5 caused the disappearance of the conjugate peaks from the chromatogram and the appearance of unconjugated I. The glucuronides of 7-hydroxycannabidiol, and probably also of 6 α -hydroxycannabidiol, were observed in the unhydrolyzed metabolic fraction. Glucuronic acid was conjugated to an aromatic rather than to an aliphatic OH group. The major in vivo metabolites of I are the glucuronides of I and 7-hydroxycannabidiol.

IT 50725-17-2D, glucuronide
 RL: BIOL (Biological study)
 (as cannabidiol metabolite, in liver)
 RN 50725-17-2 CAPLUS
 CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L17 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1977:11675 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 86:11675
 ORIGINAL REFERENCE NO.: 86:1879a,1882a
 TITLE: Dioxygenated metabolites of cannabidiol formed by rat liver
 AUTHOR(S): Martin, Bill; Agurell, Stig; Nordqvist, Marianne; Lindgren, Jan E.
 CORPORATE SOURCE: Dep. Pharmacognosy., Fac. Pharm., Uppsala, Swed.
 SOURCE: Journal of Pharmacy and Pharmacology (1976), 28(8), 603-8
 CODEN: JPPMAB; ISSN: 0022-3573
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

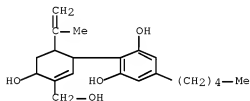


AB The 6,7-dihydroxy, 1'',7-dihydroxy, 3'',7-dihydroxy, 4'',7-dihydroxy, 5'',7-dihydroxy, 2'',6-dihydroxy, 3'',6 β -dihydroxy, 4'',6 β -dihydroxy, 3''-hydroxy-6-oxo, and 4'',hydroxy-6-oxo derivs. of cannabidiol (I) [13956-29-1] were identified as dioxygenated metabolites of I in the 10,000-g supernatant fraction of rat liver. In both the monohydroxylated and dioxygenated metabolites of I, 7-hydroxylation occurred to the greatest extent. Side-chain hydroxylation occurred predominantly at C-4'' and to a lesser degree at C-3''. Trace amts. of metabolites were hydroxylated at C-1'', C-2'', or C-5''.

IT 61361-39-5 61361-40-8 61361-41-9
61361-42-0 61361-43-1
RL: BIOL (Biological study)
(as cannabidiol metabolite, in liver)

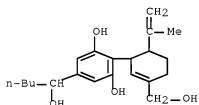
RN 61361-39-5 CAPLUS

CN 1,3-Benzenediol, 2-[4-hydroxy-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)



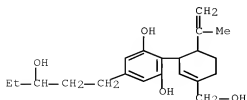
RN 61361-40-8 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(1-hydroxypentyl)- (CA INDEX NAME)



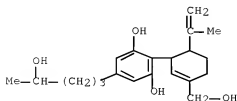
RN 61361-41-9 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(3-hydroxypentyl)- (CA INDEX NAME)



RN 61361-42-0 CAPLUS

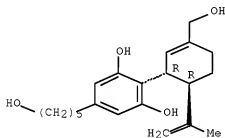
CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(4-hydroxypentyl)- (CA INDEX NAME)



RN 61361-43-1 CAPLUS

CN 1,3-Benzenediol, 2-[3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-(5-hydroxypentyl)-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:486979 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 85:86979

ORIGINAL REFERENCE NO.: 85:13859a,13862a

TITLE: Chromatographic separation of cannabinoids and their monooxygenated derivatives

AUTHOR(S): Fonseka, Kanthi; Widman, Marianne; Agurell, Stig

CORPORATE SOURCE: Dep. Pharmacogn., Fac. Pharm., Uppsala, Swed.

SOURCE: Journal of Chromatography (1976), 120(2), 343-8

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Δ^1 -Tetrahydrocannabinol (I) [1972-08-3], Δ^6 -tetrahydrocannabinol [5957-75-5], cannabinol [521-35-7], cannabidiol [13956-29-1], and several of their monooxygenated derivs. were separated from each other by a combination of liquid, thin-layer and gas chromatog. Retention vols. (on Sephadex LH-20), RF values and retention times can be recorded, and may provide guidance in the separation and identification of these known cannabinoids.

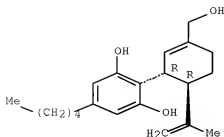
IT 50725-17-2

RL: PROC (Process)
(separation of, by chromatog.)

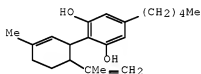
RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



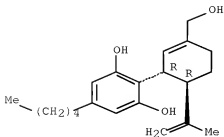
L17 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1976:471953 CAPLUS Full-text
 DOCUMENT NUMBER: 85:71953
 ORIGINAL REFERENCE NO.: 85:11483a,11486a
 TITLE: Identification of monohydroxylated metabolites of
 cannabidiol formed by rat liver
 AUTHOR(S): Martin, Bill; Nordqvist, Marianne; Agurell, Stig;
 Lindgren, Jan E.; Leander, Kurt; Binder, Michael
 CORPORATE SOURCE: Dep. Pharmacognosy, BMC, Uppsala, Swed.
 SOURCE: Journal of Pharmacy and Pharmacology (1976), 28(4),
 275-9
 CODEN: JPPMAB; ISSN: 0022-3573
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I

AB Cannabidiol (I) [13956-29-1] was metabolized by rat liver enzymes in vitro to
 7-hydroxy-I [50725-17-2] (major metabolite), 6 α -hydroxy-I [58940-28-6], and
 trace amts. of 6 β -hydroxy-I [59888-03-8]. Hydroxylation occurred in all
 positions of the pentyl side chain to give 1''- [53413-21-1], 2''- [53413-22-
 2], 3''- [42965-06-0], 4''- [59877-46-2], and 5''-hydroxy-I [53413-28-8].
 IT 50725-17-2
 RL: BIOL (Biological study)
 (as cannabidiol metabolite, of liver)
 RN 50725-17-2 CAPLUS
 CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-
 cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L17 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:35 CAPLUS Full-text

DOCUMENT NUMBER: 80:35

ORIGINAL REFERENCE NO.: 80:3a,6a

TITLE: Two cannabidiol metabolites formed by rat liver

AUTHOR(S): Nilsson, I.; Agurell, S.; Nilsson, J. L. G.; Widman, M.; Leander, K.

CORPORATE SOURCE: Fac. Pharm., Stockholm, Swed.

SOURCE: Journal of Pharmacy and Pharmacology (1973), 25(6), 486-7

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Metab. of cannabidiol (I) [13956-29-1] by rat liver homogenates did not yield Δ^1 -tetrahydrocannabinol [1972-08-3]. Two metabolites were obtained in the ratio 8:2. On the basis of mass spectroscopy and NMR one of these was assigned the structure 7-hydroxycannabidiol (II) [42965-05-9]. Thin-layer chromatog., gas chromatog., and mass spectroscopy suggested the other was 3''-hydroxycannabidiol (III) [42965-06-0].

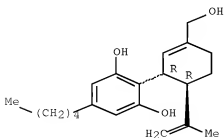
IT 50725-17-2

RL: FORM (Formation, nonpreparative)
(formation of, from cannabidiol)

RN 50725-17-2 CAPLUS

CN 1,3-Benzenediol, 2-[(1R,6R)-3-(hydroxymethyl)-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



=> LOG HOLD

(FILE 'HOME' ENTERED AT 10:00:42 ON 01 SEP 2009)

L1 FILE 'REGISTRY' ENTERED AT 10:01:06 ON 01 SEP 2009
STRUCTURE UPLOADED
D
L2 0 SEA FILE=REGISTRY SSS SAM L1
L3 1 SEA FILE=REGISTRY SSS FUL L1
L4 1 SEA FILE=REGISTRY SSS FUL L1
D L4

L5 FILE 'CAPLUS' ENTERED AT 10:02:40 ON 01 SEP 2009
0 SEA FILE=CAPLUS SPE=ON PLU=ON L4
L6 0 SEA FILE=CAPLUS SPE=ON PLU=ON L3

FILE 'STNGUIDE' ENTERED AT 10:04:28 ON 01 SEP 2009

L7 FILE 'REGISTRY' ENTERED AT 10:08:07 ON 01 SEP 2009
STRUCTURE UPLOADED
D
L8 0 SEA FILE=REGISTRY SSS SAM L7
L9 3 SEA FILE=REGISTRY SSS FUL L7
D L9 1-3

L10 FILE 'CAPLUS' ENTERED AT 10:09:28 ON 01 SEP 2009
11 SEA FILE=CAPLUS SPE=ON PLU=ON L9
D L10 1-11 IBIB ABS HITSTR

FILE 'STNGUIDE' ENTERED AT 10:12:43 ON 01 SEP 2009

FILE 'STNGUIDE' ENTERED AT 10:13:20 ON 01 SEP 2009

L11 FILE 'REGISTRY' ENTERED AT 10:17:39 ON 01 SEP 2009
STRUCTURE UPLOADED
D
L12 7 SEA FILE=REGISTRY SSS SAM L11
L13 228 SEA FILE=REGISTRY SSS FUL L11

FILE 'STNGUIDE' ENTERED AT 10:18:51 ON 01 SEP 2009

L14 FILE 'REGISTRY' ENTERED AT 10:22:42 ON 01 SEP 2009
STRUCTURE UPLOADED
D
L15 3 SEA FILE=REGISTRY SSS SAM L14
D SCAN
L16 77 SEA FILE=REGISTRY SSS FUL L14
D L16 1-77

L17 FILE 'CAPLUS' ENTERED AT 10:34:29 ON 01 SEP 2009
36 SEA FILE=CAPLUS SPE=ON PLU=ON L16
D L17 1-36 IBIB ABS HITSTR

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	204.04	1377.71
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-29.52	-38.54

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STN INTERNATIONAL SESSION SUSPENDED AT 10:35:30 ON 01 SEP 2009